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Review Article

Computational Synergetics and Mathematical Innovation*

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It is demonstrated how the computer, used in a heuristic mode, has greatly augmented our understanding of the mathematics of nonlinear dynamical process. Examples are given of recent work in soliton mathematics (mainly), but also nonlinear iterative mappings and low-order nonlinear ordinary differential equation systems. The role of good graphics in enhancing the discovery and retention of new mathematical properties of equations is illustrated. Several examples are given of the present frontier of research in two space dimensional nonlinear evolutionary problems.

1. INTRODUCTION

In the early fifties E. Fermi, the theoretical physicist, remarked that the results "... really constituted a little discovery ..." [1]. He referred to an observation of near-recurrence in numerical solutions of 32 coupled nonlinear differential equations on the MANIAC I computer at Los Alamos. This pioneering work, called the Fermi, Pasta, Ulam (FPU) problem, is an example of the heuristic use of computers which I will elaborate in this paper.

My goal is to show with concrete examples how, by the *judicious* use of computers, we can penetrate into new areas and discover linkages to diverse areas of mathematics unforeseen by our forbears. With insight obtained from numerous solutions, often displayed naturally by graphs and cinemas, we may be liberated from the prejudices of our conservative and sometimes misguided mathematical intuitions [2]. For, as Fermi continued, these results provided "... intimations that the prevalent

* This paper is dedicated to

J. von Neumann:	who foresaw what was to be;
S. M. Ulam:	who elaborated for all to see;
M. D. Kruskal:	who introduced it to me.

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beliefs in the universality of 'mixing and thermalization' in nonlinear systems may not always be justified."

As with others before me [3], I will not attempt a philosophical or psychological discussion. I will relate essentially my experiences with the FPU problem and solitons and my interpretation of the experience of E. N. Lorenz with three nonlinear differential equations and the Los Alamos group of Ulam, Stein, Metropolis and Feigenbaum on nonlinear mappings. From these, I will attempt to distill essences of a synergetic computational style.

I use the word "synergetic" here to mean the enhancement in the rate and depth of mathematical understanding through the combined use of analysis and computer simulation. "Synergetic" was first used in this context by S. M. Ulam [4]. I illustrated these general ideas in relation to the FPU problem [5] in the early soliton days prior to 1967.

In the past, I have found it difficult to relate this mode of working via lectures. Perhaps this mode is still an art form understood by committed practitioners in benign computer environments and learned only by apprenticeship. Perhaps this difficulty is related to the item in Lankavatara Sutra, "... words and sentences ... cannot express the highest reality .... Truth is beyond letters and words and books" [6]. However, I believe things are changing and in the future we will transcend these communication barriers by improving the training that scientists and engineers receive, as discussed by Davis and Anderson in a refreshing and vital paper [6].

Almost everyone using computers has experienced instances where computational results have sparked new insights. The range covered is large: from uncovering mistakes in formal derivations or calculations; to suggesting combinations of parameters with which to make asymptotic expansions and thereby obtain equations which are analytically tractable [7]; and finally to shining the light of inspiration into areas which have been thought devoid of possible new concepts or new fundamental truths. The last, namely, the heuristic use of computers to obtain and display the results of numerical experiments where parameters are varied and solutions returned in a rapid interactive fashion is the mode of working that I will elaborate.

Although several pioneering steps have been taken, we are just at the beginning of a mind-augmenting revolution that inexpensive and robust computing will allow the prepared investigator.

2. Historical Perspectives

L. F. Richardson in 1922 foresaw how computers could revolutionize the understanding and prediction of meteorological processes [8]. However, he seemed to be unaware of the complexity of physical phenomena and the magnitude of the computational problem.

John von Neumann foresaw all of it! His belief that high-speed computation would revolutionize the approach to mathematics and the way we explore, understand and

apply the natural sciences is expressed in papers that radiate inspiration [9, 10]. His beliefs were undoubtedly shaped by being deeply involved with answer-demanding applied-mathematical problems. They resulted mainly from the exigencies of World War II and the nuclear developments arising afterwards and included: shock wave compressible flow; vortical, turbulent and incompressible atmospheric flows; porous-media flows; neutron diffusion, etc.; inversion of large matrices; and the development of numerical and coding methods to obtain solutions.

In 1946 he asked: "To what extent can human reasoning in the sciences be more efficiently replaced by mechanisms?" and: "What phases of pure and applied mathematics can be furthered by the use of large-scale, automatic computing instruments?"

He continued in [9, Sect. 2], entitled "Importance to Mathematics":

> Our present analytical methods seem unsuitable for the solution of the important problems arising in connection with non-linear partial diferential equations and, in fact, with virtually all types of non-linear problems in pure mathematics. The truth of this statement is particularly striking in the field of fluid dynamics. Only the most elementary problems have been solved analytically in this field....
>
> The advance of analysis is, at this moment, stagnant along the entire front of non-linear problems. That this phenomenon is not of a transient nature but that we are up against an important conceptual difficulty ... yet no decisive progress has been make against them ... which could be rated as important by the criteria that are applied in other, more successful (linear!) parts of mathematical physics....
>
> It is important to avoid a misunderstanding at this point. One may be tempted to qualify these [shock wave and turbulence] problems as problems in physics, rather than in applied mathematics, or even pure mathematics. We wish to emphasize that it is our conviction that such an interpretation is wholly erroneous....
>
> They give us the first indication regarding the conditions that we must expect to find in the field of non-linear partial differential equations, when a mathematical penetration into this area, that is so difficult of access, will at least succeed. Without understanding them and assimilating them to one's thinking even from the strictly mathematical point of view, it seems futile to attempt that penetration....
>
> That the first, and occasionally the most important, heuristic pointers for new mathematical advances should originate in physics, is not a new or a suprising occurrence. The calculus itself originated in physics....
>
> ... we conclude by remarking that really efficient high-speed computing devices may, in the field of non-linear partial differential equations as well as in many other fields which are now difficult or entirely denied of access, provide us with those heuristic hints which are needed in all parts of mathematics for genuine progress.... This should ultimately lead to important analytical advances.

I have quoted extensively to illustrate von Neumann's originality and rare prescience [11, 12] and to justify my title.

The "stagnant" condition to which von Neumann referred was the result of the approach and collective intuition dominating mathematics. Courant and Robbins [13] also noted, "There seems to be a great danger in the prevailing overemphasis on the deductive–postulational character of mathematics...." and Hahn [14] remarks, "... intuition is force of habit rooted in psychological inertia," or the preservation of "self." It is not surprising that breakthroughs in the areas outlined

by von Neumann were accomplished mainly by young physicists and applied mathematicians often working at, or in collaboration with, laboratories that have pioneering practical responsabilities.

Heisenberg contributed his experiences with strongly interacting physical phenomena at the first International School of Nonlinear Physics [15]. He noted, "... the progress of physics will to a large extent depend on the progress on nonlinear-mathematics, of methods to solve nonlinear equations ... and therefore one can learn by comparing different nonlinear problem." S. M. Ulam, was also intrigued by nonlinear phenomena and their natural appearance in physical and biological systems. In his 1960 monograph, "A Collection of Mathematical Problems" [4] he points to two areas that he and his colleagues considered, namely, the problem of oscillations in a nonlinear one-dimensional lattice of equimass particles (the FPU problem) and the problem of nonlinear transformations or iterative mappings.

The major part of this paper is devoted to the FPU problem and solitons because of: remarkable mathematical developments; numerous applications in diverse areas of physics; and the emergence of a new style of working. In Section 3 our discussion moves between discrete and continuous representations of physical systems and is divided into three chronological periods: early (until 1964); heroic (1965–1971); and generalization, abstraction, and application (1972–present). The discussion will be punctuated with "Remarks" which are commentaries to highlight aspects of the narrative. As will be seen, computer simulation plays a major probing role during the first period; a strong synergetic role during the second period; and a necessary supporting role during the last period.

In Section 4 we look at the panorama of new directions. In Section 4.1 we review recent progress in nonlinear lattice dynamics. In Section 4.2 we look at few-mode nonlinear systems and universal behavior that may be relevant to continuous systems. In Section 4.3 we review pioneering studies by computational physicists and mathematicans of the interaction of localized states in two-space dimensions. Again, the computer's primacy is ascendant, for we are moving out of the (x, t) flatlands into the domain where integrable systems are less prevalent. Finally, in Section 4.4 we consider the shallow water wave milieu. We examine the role of modeling, analysis, and experiment, as synergized by computation in elucidating natural phenomena.

3. Fermi–Pasta–Ulam Problem and Solitons

3.1. *The Early Period (until 1964)*

Physicists since early times wrestled with the problem of the transport of heat in nonlinear (or "anharmonic") solids. Debye [16] in 1914 suggested that the finiteness of the thermal conductivity of an anharmonic (or nonlinear) nonconducting lattice was due essentially to its nonlinearity. In other words, he suggested that the phonons or fundamental wave propagation modes would interact because of the nonlinearity, thereby inhibiting the propagation of energy. The net effect of many such nonlinear

interactions or "phonon collisions" would manifest itself in a finite thermal transport coefficient; that is, if there is a "mean" energy flux through a region, there will be an energy gradient across this region.

The problem of deducing a finite thermal conductivity for an anharmonic lattice from its microscopic properties has challenged theoretical physicists for the last fifty years, and as Peierls [17] observed in his penetrating review paper, "It seems there is no problem in modern physics for which there are on record as many false starts, and as many theories which overlook some essential feature, as in the problem of the thermal conductivity of nonconducting crystals." It is undoubtedly this unsatisfactory state of affairs which motivated Fermi, Pasta, and Ulam [18] to undertake a numerical study of the one-dimensional nonlinear lattice. Rather than examine the flow of energy from one thermal bath to another bath at lower temperature (we return to this problem below), they posed a simpler but related problem: How would a long-wavelength initial condition relax in a nonlinear dissipationless medium? Fermi and Ulam had been interested in the ergodic behavior of mathematical and physical systems, including problems associated with iterative mappings and the rate of approach and the asymptotic spectrum associated with energy partition in Hamiltonian systems, etc. "Stochastic" and "chaotic" are also employed as adjectives for turbulent-like behavior.

They believed that many-body nonlinear systems would exhibit a relaxation time and this physical intuition or hypothesis led FPU to set up a computational program that represents in our case the beginning of the synergetic approach for this mathematical model. For convenience in presentation, we designate it as Hypothesis 1 or H1 and summarize it by:

H1. *Given a one-dimensional lattice with fixed boundary conditions and with identical nearest neighboring masses coupled by identical nonlinear springs. If the energy of the system is initially in a long-wavelength state, the energy will eventually be shared "equally" among all the degrees of freedom of the system.*

We anticipate future work in this field by noting that Hypothesis 1 restricts the problem and thus the resulting solutions by being: specific with respect to the dimensionality, boundary conditions and masses of the system; somewhat specific with respect to the initial conditions; and vague with respect to the type of nonlinearity selected. Figure 1 depicts the system of identical masses m with equilibrium separation

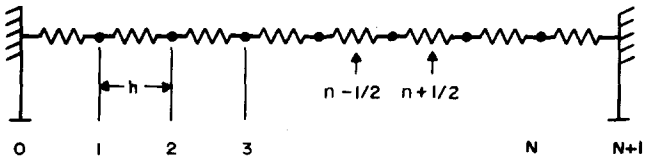


FIG. 1. A one-dimensional lattice with fixed boundary conditions and neighboring masses coupled by nonlinear springs.

h and length $L = (N+1)h$. Two of the three cases studied dealt with power-law nonlinearities, namely, where the energy stored in spring $(n, n+1)$ was

$$V_{n+1,n} = \tfrac{1}{2}\kappa(y_{n+1} - y_n)^2 + \kappa\alpha(y_{n+1} + y_n)^{p+2}/(p+2), \tag{1}$$

where $(y_{n+1} - y_n)$ is the displacement and the energy of the system is

$$H = H_L = H_{NL},$$

where

$$H_L = \sum_{n=1}^{N} \tfrac{1}{2}m\dot{y}_n^2 + \tfrac{1}{2}\kappa(y_{n+1} - y_n)^2 = \sum_{k=1}^{N} E_k^{(L)}, \tag{2a}$$

and

$$H_{NL} = \kappa\alpha \sum_{n=1}^{N} (y_{n+1} - y_n)^{p+2}/(p+2). \tag{2b}$$

The last sum in (2a) is over modes, where

$$E_k^{(L)} = \tfrac{1}{2}(\dot{a}_k^2 + \omega_k^2 a_k^2), \tag{3}$$

and $a_k = a_{-k}$ are the spatial modes of the system defined by

$$a_k(t) = \sum_{n=1}^{N} y_n(t)\, e^{-ikn\pi/N} \qquad (k = 0, 1, \ldots, N), \tag{4}$$

and

$$\omega_k^2 = 4\omega_0^2 \sin^2(k\pi/2N), \tag{5}$$

where $\omega_0^2 = (\kappa/m)^2$ is the resonant frequency of a linear sping-mass system.

For $p = 1$ and 2 we have the so-called "cubic" and "quartic" nonlinearities, respectively. When p is odd, there exists the unphysical possibility of "blow-up," namely, where the energy density ceases to increase with increasing displacement $(y_{n+1} - y_n)$. To avoid this possibility we constrain our initial condition to

$$\alpha\,|(y_{n+1}(0) - y_n(0))|^p < \tfrac{1}{2} \tag{6}$$

for p odd. For $p = 2$, one can obtain two minima of potential energy if $\kappa < 0$ and $\alpha\kappa > 0$, that is, two stable equilibria. Thus, it is clear that with simple structures such as (1) there are a host of interesting problems to study. Below we will return to a discussion of other forms of the potential energy, either to have a physically relevant model for strong excitations or to obtain a mathematically tractable model.

The equations governing the dynamics of the FPU lattice are

$$\omega_0^{-2}\ddot{y}_n = (y_{n+1} - 2y_n + y_{n-1}) + \alpha[(y_{n+1} - y_n)^{p+1} - (y_n - y_{n-1})^{p+1}], \qquad (7)$$
$$n = 1, 2, \ldots, N \qquad \text{and} \qquad y_0 = y_{N+1} = 0,$$

where $y_n \equiv y_n(t)$ is the displacement of the nth mass from its equilibrium position.

To solve (7), FPU discretized the left side with

$$\ddot{y}_n \to [y_n(t + \Delta t) - 2y_n(t) + y_n(t - \Delta t)]/(\Delta t)^2, \qquad (8)$$

where Δt was the time step and $\omega_0(\Delta t) \leqslant \sqrt{0.8}$. For $p = 1$, (7) takes the form

$$\ddot{y}_n = \omega_0^2(y_{n+1} - 2y_n + y_{n-1})[1 + \alpha(y_{n+1} - y_{n-1})], \qquad (9)$$
$$n = 1, 2, \ldots, N \qquad \text{and} \qquad y_0 = y_{N+1} = 0,$$

and FPU chose the lowest-mode initial condition

$$y_n|_0 = a \sin(n\pi/N), \qquad \dot{y}_n|_0 = 0. \qquad (10)$$

Much to their surprise, the system did not "equilibrate" energy among all the N-modes of the system, but rather exhibited long-time near-recurrences and energy sharing only among the lowest modes of the system. This is shown in the modal plot of Fig. 2 [18], where we observe the mode 1 energy $E_1^{(L)}$ flowing to several other modes and finally returning *almost* completely to mode 1 after 158 linear periods or one *near*-recurrence period, t_R. Although FPU varied N from 16 to 64 and α from $\frac{1}{4}$ to 1, they found no qualitative difference in the model behavior; only the recurrence time and low-mode amplitudes varied, as discussed earlier [19]. Namely, I fitted data from five runs and obtained the formula

$$t_R/t_L = 1.4(N^3/\alpha)^{1/2}. \qquad (11)$$

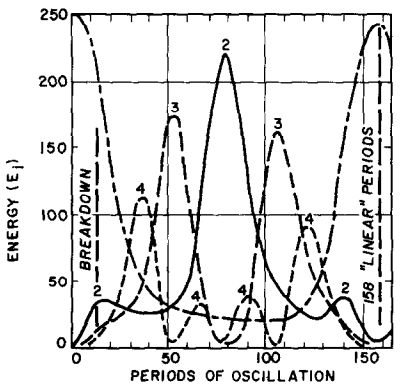


FIG. 2. The modal energies in arbitrary units (proportional to $E_k^{(L)}(t)$). The "cubic" lattice of Fig. 1 with $N = 32$, $\alpha = \frac{1}{4}$ and $a = 1$ in Eq. (10).

Here $t_L = 2/c_L$ is the time required for one oscillation of the corresponding linear string ($\alpha = 0$).

So, for the parameter configuration and initial conditions, Hypothesis 1 is not true. One could be concerned with the lack of an equilibration state and attempt to force it on the system, either through a modification of the spring and mass constants or by the appeal to one's physical intuition, that real three-dimensional crystals have many more degrees of freedom and, therefore, more available trajectories in phase space. Let us, however, follow the heuristic direction indicated by the computer solutions and seek an answer to the near-recurrence problem. Is there something essentially new in a mathematical–physical context or is it only a mathematical nonessential resulting from the manner in which we discretized time or applied our boundary conditions? Perhaps it is a combination of both?

There are several ways of proceeding toward a global or detailed analytic understanding of this phenomenon. A mathematical approach to the generic properties of classical *discrete* Hamiltonian systems has been started by G. D. Birkhoff, K. Siegel, A. N. Kolmogoroff, V. I. Arnold, J. Moser, and Ya. G. Sinai and many others in recent years [20]. Kolmogoroff, Arnold, Moser, and Siegel (KAMS) have proved theorems that show: If one obtains a nonintegrable system by "weakly" perturbing the structure of an integrable system, then there still remain parameter regions where the quasiperiodic solutions of the integrable system persist. That is, with an appropriate choice of initial data, "invariant torii" of integrable systems may not be destroyed under a weak structural perturbation (i.e., a modification of the equations or boundary conditions). Although nonintegrable, the cubic lattice with appropriate initial conditions yields solutions that are "close" to solutions of integrable systems, like the Toda lattice, as described below.

A second "continuum" or partial differential equation approach may be adopted because we observe that only the low modes of the system participate in the dynamics. This assumption was first presented by M. D. Kruskal in 1960 in a stimulating seminar on unsolved mathematical–physical problems [21]. He discussed the "breakdown" paradox [22] (also discussed below) which prompted me to join him to unravel the FPU problem, and we are led to Hypothesis 2.

H2. *The near-recurrence phenomenon and the detailed modal history can be explained by a continuum model.*

We assume that the displacements $y_{n\pm1}$ can be written in terms of the displacement y_n and its derivatives by means of the Taylor series

$$y_{n\pm1} \to [y \pm hy_x + (h^2/2)y_{xx} \pm (h^3/6)y_{xxx} + (h^4/24)y_{xxxx} + 0(h^5)]|_{x=nh}. \quad (12)$$

If we substitute in (9) we obtain

$$c_L^{-2}y_{tt} = (1 + \varepsilon y_x)y_{xx} + (h^2/12)y_{xxxx} + (\varepsilon h^2/6)y_{xxx}y_{xx} + O(h^4) + O(\varepsilon h^4), \quad (13)$$

where $\varepsilon = 2\alpha h$ and $c_L^2 = h^2\omega_0^2$ is the propagation speed of waves in the lowest continuum linear limit, viz., $\varepsilon = h = 0$. In our case we normalize the length of the

lattice so that $L = (N+1)h = 1$. If $\alpha = O(1)$, then $\varepsilon = O(h) \gg h^2$, and the *lowest* continuum limit is the nonlinear hyperbolic partial differential equation

$$y_{tt} = c_L^2(1 + \varepsilon y_x)\, y_{xx}. \tag{14}$$

The initial–boundary conditions corresponding to the FPU problem are

$$y(x, 0) = a \sin \pi x, \qquad y_t(x, 0) = 0, \qquad y(0, t) = y(1, t) = 0. \tag{15}$$

Remark 1. *Temporal discretization.* FPU noted that the recurrence time varied if (Δt) in Eq. (8) varied. This can be explained by taking the continuum limit of (8). The leading truncation error term is $(\Delta t)^2/12)\, y_{tttt} \propto (c_L^4(\Delta t)^2/12)\, y_{xxxx} + \cdots$. Thus, to lowest order, temporal discretization modifies the coefficient of the fourth spatial derivative. ∎

Kruskal assumed periodic boundary conditions for (14) and by a heuristic asymptotic derivation, he obtained the first-order hyperbolic equation

$$r_t + c_L(1 + \varepsilon r/2)\, r_x = 0, \tag{16}$$

where, to zero order,

$$r = \tfrac{1}{2}(\pm c_L^{-1} y_t + y_x) + O(\varepsilon). \tag{17}$$

If we transform to a coordinate system moving with velocity c_L and substitute

$$\tau = \varepsilon c_L\, t/2, \qquad \xi = x - c_L\, t$$

we obtain

$$r_\tau + r r_\xi = 0. \tag{18}$$

Equation (18) can be solved by the method of characteristics as the implicit function

$$r = R(\xi - r\tau), \tag{19}$$

where

$$r(\xi, 0) = R(\xi).$$

The ξ derivative of r is

$$r_\xi = R'/(1 + \tau R') \tag{20}$$

and the denominator vanishes when $\tau_B = \min(R')$ if $\min R' < 0$. Thus, the third and higher derivatives (which were omitted in writing (16)) become singular in a finite time. That is, the solution "breaks down." The normalized breakdown time is

$$t_B/t_L = 2/\varepsilon a \pi^2, \tag{21}$$

or it is inversely proportional to the ratio of the nonlinear to the linear term. The only evidence that something occurred at this time in the modal energy diagrams of FPU was a local maximum of the second harmonic, as seen in Fig. 2.

Remark 2. *Discrete or continuous model.* Equation (14) is really the one that FPU had in mind for their investigation. On the first page of their classic paper [18, p. 979] they say, "We imagine a one-dimensional continuum... . For the purposes of numerical work this continuum is replaced by a finite number of points (at most 64 in our actual computation) so that the partial differential equation defining the motion of this string is replaced by a finite number of total differential equations." Also, FPU did not realize that the continuum representation would not describe the discrete representation for all times. In fact, in their original memo they presented graphs of $y_n(t)$ vs n and not $(y_{n+1} - y_n)$ vs n, which would have been much more suggestive of the breakdown phenomena. Ornstein and Zernike in 1914 [23] used (14) to study the thermal conductivity problem by perturbation methods, without much success. ∎

This behavior raises three questions related to modifications of the equation and boundary conditions:

(1) Does the second-order hyperbolic equation (14) with fixed or periodic boundary conditions exhibit breakdown in a finite time?

(2) Does the lattice problem with *periodic* boundary conditions exhibit solutions similar to those of the fixed boundary problem?

(3) How must one modify the lowest continuum equations to model the lattice solutions beyond breakdown?

The first two questions were answered in the affirmative, the first by analysis and the second by computation.

In 1962 [24], I used the hodograph transformation to linearize (14) exactly and obtained the Euler–Poisson–Darboux partial differential equation. In an involved calculation, I was able to prove the existence of breakdown. With this insight P. D. Lax [25] presented in 1964 a simpler analysis and showed the conditions for breakdown for the class of equations

$$y_{tt} - F(y_x)\, y_{xx} = 0.$$

The discussion of breakdown has now become a branch of analysis for systems of nonlinear hyperbolic differential equations.

In December 1962, at the American Physical Society meeting in Standord California, I presented the first calculations for the lattice with *periodic* boundary conditions. I showed the modal diagrams which answered question 2 in the affirmative; namely, it showed near-recurrence and the property that the location of the maxima of the prime numbered modes, n_p, divides *approximately* the interval t_R/t_L into n_p parts. This is evident in Fig. 2 for $n_p = 2, 3$ and in [19] for $n_p = 2, 3, 5, 7, 9$. I also showed Figs. 3a, 3b and 3c (not heretofore published) which were motivated by

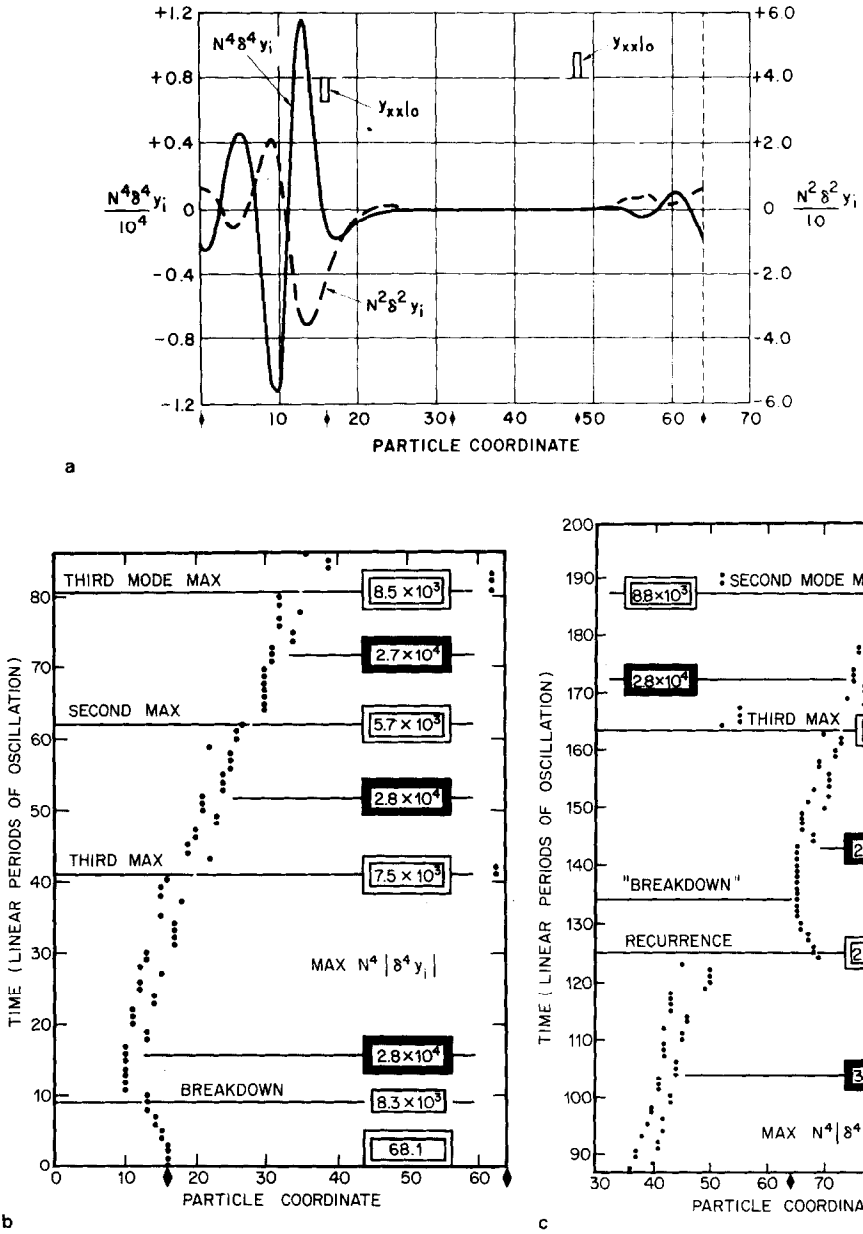


FIG. 3(a). Waveforms of $(\delta^2 y_n/10h^2)$ and $(\delta^4 y_n/10^4 h^4)$ vs n at $t = 10$, for the cubic lattice with periodic boundary conditions and $N = 64$. The value of the minimum and maximum of $(\delta^2 y_n/10h^2)$ at $t = 0$ and $n = 16$ and $n = 64$ is shown by the rectangle below and above 0.8. (b) Trajectory of the Max $|\delta^4 y_n/10^4 h^4|$ vs n for $0 \leqslant t \leqslant 85$. For the cubic lattice with periodic boundary conditions and $N = 64$. (c) Continuation of Fig. 3b. Note that the horizontal and vertical scales of (c) are different from those of (b) and they are displaced.

the breakdown phenomena. Namely, if $y_x \propto r$ becomes singular for solutions of (9) and (10) then the discrete analog of y_{xx} and y_{xxx} should also become large. Thus, we plotted $(\delta^2 y_n/10h^2)$ and $(\delta^4 y_n/10^4 h^2)$ vs n at $t = 10$ (breakdown) and the maxima and minima of $y_{xx}|_0 \propto (\delta^2 y_n/h^2)$ for comparison. It is evident that $\delta^2 y_n/h^2$ has grown by a factor of 40. We anticipated some kind of "nonlinear wave," and plotted the location of Max $|\delta^4 y_n/h^4|$. The breakdown and recurrence times are labelled as well as the time of second- and third-mode maxima. In the rectangular boxes, we see the values of Max $|\delta^4 y_n/h^4|$ grow from 68.1 at $t = 0$ to a maximum of 2.8×10^4. After breakdown we see the trajectory has an average velocity to the right with interludes where the velocity is zero and small intervals where there is an apparent large rightward velocity (or "phase shift"). In retrospect, the qualitative features of this trajectory diagram can be explained in terms of the soliton concept discussed below. However, at that time all we had was an estimate of the velocity of the leading "nonlinear" wave. Note that Figs. 3b and c differ in scales so comparison is awkward. Also note that we have only near-recurrence; that is, Max $|\delta^4 y_n/h^4|$ did not drop below 2.1×10^3.

Remark 3. *Synergetics and graphics.* I emphasize here that the benefits of the synergetic approach are dependent on the type of graph drawn. As in a laboratory experiment, one must be alert to recognize small effects that may signal new phenomena. Often one views the results of a computation according to some preconceived "intuition." Generally, I have found, for these nonlinear dispersive wave problems or where coherent entities interact and preserve some of their a priori state (e.g., in vortex dynamics), that the description according to interacting normal modes (or global basis functions) is unrewarding for making decisive progress. Following the trajectory of extrema can be very useful although sometimes the picture is confused because of large amounts of "noise." In Remark 7 we return to a more complete review of graphics and software. ∎

As for the third question, I suggested [19, Sect. 6] that the fourth derivative term alone in the continuum expansion for (9) could account for the recurrence time. This suggestion was based on a parameter-balance argument from which a recurrence time that scaled like (11) was obtained. Thus, we focussed our attention on the partial differential equation

$$0 = c_L^{-2} y_{tt} - (1 + \varepsilon y_x)\, y_{xx} - (h^2/12)\, y_{xxxx}. \tag{22}$$

We emphasize that this additional term is the first term in an expansion that takes into consideration the discreteness of graininess of the medium. As noted in Remark 1 the coefficient of y_{xxxx} does not include the effect of time discretization. Note that the linearized form of (22) represents a dispersive medium with dispersion relation

$$(\omega^2/c_L^2) = k^2 - (h^2/12)\, k^4.$$

For $k > (12)^{1/2} h^{-1}$, $\omega^2 < 0$ and unstable modes arise as described in Remark 8.

However, it is inappropriate to consider these large wavenumbers in a model obtained by assuming a long-wavelength expansion. That is, if small-wavelength states arise from nonlinear interaction, the model must be revised.

At this stage, Kruskal and I applied some of the ideas contained in his work on an asymptotic theory for Hamiltonian systems having almost periodic solutions [26], and we developed a uniform asymptotic method for treating equations like (14) [27].

To study (22), we introduce quantities which were the Riemann invariants of (14), namely,

$$\begin{aligned} r_{\pm} &= \tfrac{1}{2}\{\pm c_L^{-1} y_t + \tfrac{2}{3}\varepsilon^{-1})[(1+\varepsilon y_x)^{3/2} - 1]\}, \\ &= \tfrac{1}{2}\{\pm c_L^{-1} y_t + y_x + (\varepsilon/4) y_x^2 + \cdots\}, \end{aligned} \tag{23}$$

and obtain the coupled equations

$$c_L^{-1}(r_{\pm})_t \mp [1 + \tfrac{1}{2}\varepsilon(r_+ + r_-)](r_{\pm})_x \mp (h^2/24)(r_+ + r_-)_{xxx} = O(\varepsilon^2) + O(\varepsilon h^2). \tag{24}$$

If we take $r_+|_0 = 0$ and assume $r_-|_0$ is a function having zero mean, it can be shown that r_+ is always $O(\varepsilon^2)$. Thus, we can omit it from (20) and we are left with a third-order equation for $r_- \equiv u$. If we transform into a frame of reference moving uniformly with velocity c_L, that is, $x \to (x - c_L t)$ and $t \to \tau$, we obtain the Korteweg–de Vries (KdV) equation

$$u_\tau + u u_x + \delta^2 u_{xxx} = 0, \tag{25}$$

where

$$\tau = \varepsilon c_L t/2 \qquad \text{and} \qquad \delta^2 = h^2/12\varepsilon. \tag{26}$$

This equation was first obtained by Korteweg and de Vries as the quintessential equation for describing long-wave propagation on shallow water [28]. Gardner and Morikawa [29] rederived this equation and also showed that it was the limiting equation for describing long-wave propagation perpendicular to a uniform magnetic field in a cold lossless (collisionless) plasma. Since 1963, many investigators, e.g., [30] have derived the KdV equation as the relevant long-wave asymptotic description of a more complete set of model equations. (See J. W. Miles' historical essay on the KdV equation [31].)

For fixed initial conditions, the solutions are a one-parameter family, e.g., δ^2. The equation is sometimes written with the parameter suppressed, or

$$u_t - 6 u u_x + u_{xxx} = 0, \tag{27}$$

and the "amplitude" of the initial condition is the parameter. The number δ^{-2} is a dispersion number in analogy with the Reynold's number of dissipative hydrodynamics. Earlier, F. Ursell [32] noted that this number played a role in

resolving the Stokes paradox with respect to nonstationary surface water waves. Note, if one includes surface tension, δ^2 may change sign.

This brings us to Hypothesis 3.

H3. *The Korteweg–de Vries equation*

$$u_t + uu_x + \delta^2 u_{xxx} = 0 \tag{28}$$

can describe propagation of small-but-finite amplitude long waves on a lossless "cubic" lattice excited by a progressive wave initial condition.

This equation is the simplest nonclassical nonlinear partial differential. The Burgers' equation

$$u_t + uu_x = \mu u_{xx}$$

is parabolic and was solved exactly by Hopf [33] and Cole [34] in the early fifties with a transformation $\phi = \exp[\int^x d\xi\, u(\xi, \tau)]$ that yielded an equivalent linear diffusion equation in ϕ. Could we find an exact solution to the KdV equation? It seemed rather difficult because of the wave-like nature of the equation. We knew several facts. First, we could write (28) in conservation form, $T_t + X_x = 0$, or

$$0 = (u)_t + [\tfrac{1}{2}u^2 + \delta^2 u_{xx}]_x,$$
$$0 = (\tfrac{1}{2}u^2)_t + [\tfrac{1}{3}u^3 + \delta^2(uu_{xx} - \tfrac{1}{2}u_x^2)]_x.$$

The first is obtained by inspection and the second if we multiply (25) by u and integrate by parts. Second, we knew of the localized stationary solution

$$u(x, t) = U(x - ct) = u_0 + A\ \mathrm{sech}^2[(x - ct)/\Delta], \tag{29}$$

where

$$c = u_0 + A/3 \qquad \text{and} \qquad \Delta^2 = 12\delta^2/A, \tag{30}$$

and of the periodic solutions, the so-called "conoidal waves." We tried to apply straightforward perturbation methods without much success.

We then turned to a numerical simulation of (28) with periodic boundary conditions and with an initial condition corresponding to a long progressive wave on the lattice. We used a "leap-frog" numerical scheme which conserves momentum and "almost" conserves energy (more about numerical algorithms in Remark 6). We found near-recurrence and very good agreement with the modal energies of the cubic lattice equations (including the fact that prime-numbered modes divide the recurrence interval into nearly equal parts). These results were reported by M. D. Kruskal in 1963 [35] without much understanding of details or of the "why" of recurrence.

REMARK 4. *Numerical asymptotics.* We have found close agreement between *numerical* solutions of two systems, the latter (KdV) being derived from the former

(cubic lattice) by an asymptotic procedure. It would be interesting to run both systems for many near-recurrence periods and examine the divergence of the solutions. Tuck and Menzel [36] did this for the cubic lattice and observed that the near-recurrence of the first-mode energy became poorer. However, after 7 near-recurrence intervals the process reversed and after 14 intervals the first-mode energy was larger than after the first near-recurrence interval. We note, as discussed below, that the KdV equation is an integrable Hamiltonian system whereas the cubic lattice has not been shown to have this property. Thus, eventually, one expects the cubic lattice to show energy equipartition among all the modes [37].

G. S. Deem had recently joined Bell Labs at Whippany and assisted us with the programming and graphics. Although we pored over numerous polar diagrams of modal energy vs modal phase they told us little of what was happening. So we began to study waveforms of $u(x, t)$ and $u_x(x, t)$ and quickly realized the essential—namely, the *solitary-wave* solution (29) was the entity dominating the evolution of the waveform. These coherent entities "emerged" from the cosine initial stated and oftentimes "merged" with others of different amplitude to form smooth regions which proceeded to decompose again into the same coherent entities which had assembled to form the smooth region.

3.2. *The Heroic Period* (1965–1971)

In 1965, we published these results [38] and Fig. 4 contains waveforms of u and Fig. 5 contains the trajectory of maxima of the waveforms to a time slightly greater than $\frac{1}{2}t_R$. M. Toda [39, Sect. 2.7] reconstructed the interval from $\frac{1}{2}t_R < t < t_R$, giving a more pleasing view. (A detailed examination of the trajectories of maxima in the vicinity of t_R and the waveforms at t_R, $2t_R$ and $4t_R$ was recently given by K. Abe and T. Abe [40].) The solid lines of Fig. 4 show the crests of these waves when they are discernible. When they interact with others they "accelerate or decelerate" giving a phase shift. The remarkable stability induced us to call them "solitons" for they seemed to have an intrinsic identity. These results were so dramatic that Deem and I summarized them in a computer-generated cine-film [41]. It's now in the Bell Labs

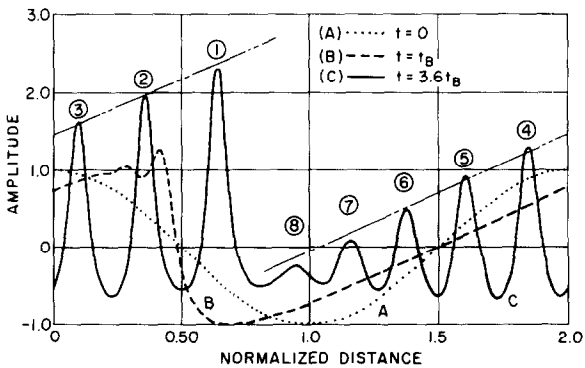


FIG. 4. Solutions of the Korteweg–de Vries equation ($\delta = 0.022$) at three different times.

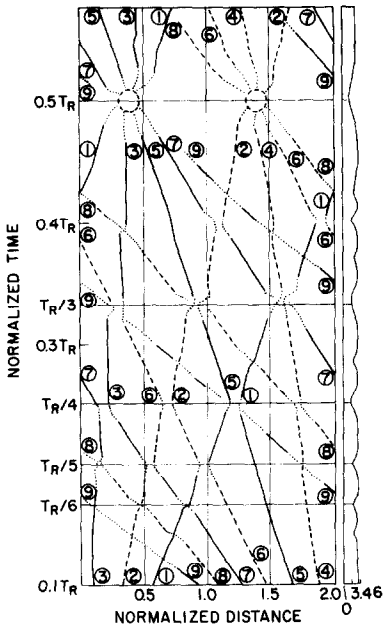


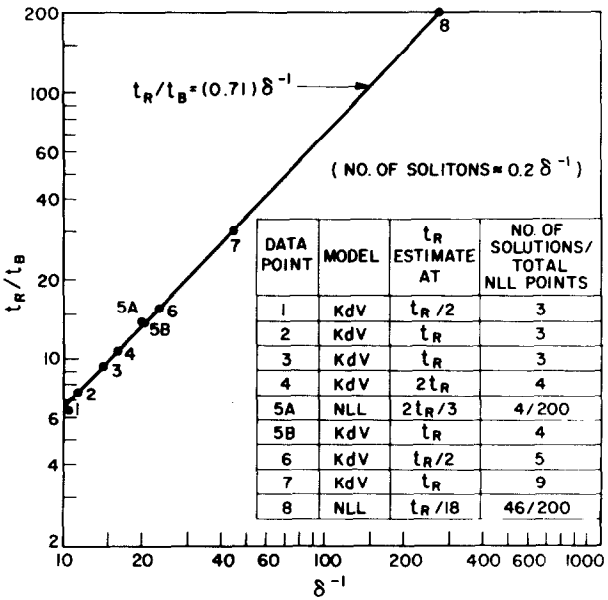
FIG. 5. Trajectories of maxima of the Korteweg–de Vries equation ($\delta = 0.022$) on a space-time diagram beginning at $t = 0.1\ t_R = 3.04 t_B$.

film library and I believe it has been and will continue to be a source of inspiration to researchers and students.

A soliton is now defined as *a localized or solitary entity that propagates at a uniform speed and preserves its structure (or shape) and speed in an interaction with another such solitary entity.* The result of such an interaction is usually a phase shift. To further determine the validity of the soliton concept, we performed scattering experiments with two well-separated solitons. For convenience, we used periodic boundary conditions and observed interactions with phase shifts and the return to initial shapes and speeds [5]. In a rigorous analysis, P. D. Lax [42] delineated the amplitude ratio regimes for two interacting KdV solitons.

F. D. Tappert and R. H. Hardin, then colleagues at Bell Labs, produced numerous films with δ^2 varying over a factor of 100. They used a split-step Fourier algorithm [43] suited to problems with periodic boundary conditions. The top of each frame contains two periods of the waveform and the lower part contains 10 decades of the Fourier transformation of u^2. Their data and other lattice results allowed us to obtain Fig. 6, t_R vs δ^{-1} [44], which showed again the correspondence of the cubic lattice with the KdV. A crude estimate was made of the recurrence time by considering the exchange and focussing of solitons on a line [45]. This estimate was improved by M. Toda [39], who included phase shifts.

Since FPU also solved the "quartic" lattice and observed near-recurrence, it



DATA POINT	MODEL	t_R ESTIMATE AT	NO. OF SOLUTIONS/ TOTAL NLL POINTS
1	KdV	$t_R/2$	3
2	KdV	t_R	3
3	KdV	t_R	3
4	KdV	$2t_R$	4
5A	NLL	$2t_R/3$	4/200
5B	KdV	t_R	4
6	KdV	$t_R/2$	5
7	KdV	t_R	9
8	NLL	$t_R/18$	46/200

FIG. 6. Normalized recurrence time as a function of dispersion parameter for the Korteweg–de Vries equation (KdV) and the cubic lattice (NLL).

seemed reasonable to solve the asymptotic representation for progressive waves, namely, the "modified" KdV (mKdV) equation

$$u_t + u^p u_x + \delta^2 u_{xxx} = 0 \qquad (p = 2). \tag{31}$$

We used periodic boundary conditions and studied the interaction of compressive ($A_1 = 1.0$) and rarefactive ($A_2 = -0.667$) solitary entities,

$$u_i = A_i \operatorname{sech}((x - c_i t)/\Delta_i), \tag{32}$$

where

$$\Delta_i = 6^{1/2}\delta/A_i \qquad \text{and} \qquad c_i = A_i^2/6. \tag{33}$$

The algorithm is described in Appendix A. The waveform results were also shown in the cine-film [41] and the trajectories of extrema are given in Fig. 7 (not previously published). Note the phase shifts. This is a demanding numerical calculation for the compressive mKdV soliton becomes taller and narrower during this interaction, unlike the KdV solitons which become wider and smaller during interaction.

At this time we became aware that G. B. Whitham had obtained a third conservation form for the KdV equation [46],

$$0 = (\tfrac{1}{3}u^3 - \delta^2 u_x^2)_t + [\tfrac{1}{4}u^4 + \delta^2(u^2 u_{xx} - 2uu_x^2) + \delta^4(-2u_x u_{xxx} + u_{xx}^2)]_x. \tag{34}$$

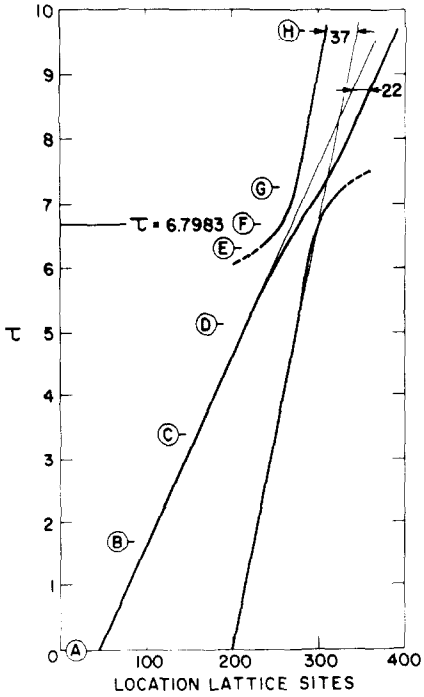


FIG. 7. Trajectories of extrema for the interaction of two solitons of the modified KdV equation (31) with $A_1 = 1.0$, $A_2 = -0.667$ in Eq. (32).

So we began to look for and found two more conserved quantities

$$T^{(4)} = \frac{u^4}{4} - 3\delta^2 u u_x^2 + \frac{9}{5}\delta^4 u_{xx}^2, \tag{35}$$

$$T^{(5)} = \frac{1}{5}u^5 - 6\delta^2 u^2 u_x^2 + \frac{36}{5}\delta^4 u u_{xx}^2 - \frac{108}{35}\delta^6 u_{xxx}^2. \tag{36}$$

R. Miura joined us in this effort and he was able to find five additional conserved quantities. There seemed to be no end. Also, we found that the mKdV had five conservations laws and the generalized KdV, (31) with $p = 3, 4,...,$ had only three conservation laws; that is, they are nonintegrable.

The environment prepared by the confluence of these analytical and computational results and the stimulation provided by Clifford Gardner, John Greene, and Martin D. Kruskal at the Plasma Physics Laboratory induced Robert Miura to assert the next analytical hypothesis.

H4. *There exists a transformation between the KdV and mKdV equations.*

After much formal algebraic manipulation, he found the beautiful transformation that hailed "open sesame" to the gates hiding the wonderland of solitons. He was able to prove [47].

THEOREM. *If v is a solution of the modified KdV equation*

$$Q(v) \equiv v_t - 6v^2 v_x + v_{xxx} = 0 \tag{37}$$

then

$$u = v^2 + v_x \tag{38}$$

is a solution of the KdV equation

$$P(u) \equiv u_t - 6uu_x + u_{xxx} = 0. \tag{39}$$

Direct substitution yields

$$Pu = [2v + \partial_x]\, Qv. \tag{40}$$

So if $Q(v) = 0$ then u satisfies the KdV equation.

Transformation (38) is analogous to the Hopf–Cole transformation for linearizing Burgers' equation, except that we are transforming between two nonlinear equations, neither of which is apparently solvable. Is it possible to use the transformation to gain insight into the analytical solution of the KdV equation?

Using this transformation, Gardner and co-workers [48], in an ingenious proof, showed the existence of an infinite number of conservation laws. To accomplish this he generalized (38) to

$$u = w + \varepsilon w_x + \varepsilon^2 w^2, \tag{41}$$

where the parameter ε has been introduced and w satisfies the *Gardner equation* [49]

$$Rw \equiv w_t - 6(w + \varepsilon^2 w^2)\, w_x + w_{xxx} = 0, \tag{42}$$

if u satisfies the KdV equation. Proceeding by substitution we find

$$0 = Pu = [1 + \varepsilon\partial_x + 2\varepsilon^2 w]\, R(w), \tag{43}$$

where $R(w)$ need not be zero because of the additional term. Since w depends on x, t, and ε we can write a formal power series for w

$$\begin{aligned} w(x, t; \varepsilon) &= w_0 + \varepsilon w_1 + \varepsilon^2 w_2 + \cdots, \\ &= u - \varepsilon u_x + \varepsilon^2 (u^2 - u_{xx}) + \cdots. \end{aligned} \tag{44}$$

Now, a formal power series solution of (43) for $R(w)$ yields

$$Rw = w_t + [-3w^2 - 2\varepsilon^2 w^3 + w_{xx}]_x \tag{45}$$

to all powers in ε. Substituting (44) into (45) yields a conservation law for the KdV equation as the coefficient of each power of ε and there is an infinite sequence of such terms. Note by this procedure they also established an infinite sequence of conservation laws for the mKdV and Gardner equations.

With this information the barriers to the analytical domain vanished. After a flourish of activity, the KdV equation was transformed to an isospectral eigenvalue problem [50], [51]. That is, (38) is a Riccati equation in v and if

$$v = \psi_x/\psi \tag{46}$$

then it linearizes to

$$\psi_{xx} - u\psi = 0.$$

Since the KdV equation is Galilean invariant, we may insert a constant (corresponding to a transformation to uniformly moving frame of reference) and obtain the eigenvalue problem

$$\psi_{xx} + (\lambda - u(x, t))\psi = 0, \tag{47}$$

where u is a potential in which t is a parameter. One finds that the discrete eigenvalues λ_n (and the remainder of the spectrum) remain *invariant* if u evolves according to the KdV equation. Each λ_n corresponds to a soliton amplitude and the properly normalized $|\psi_n|^2$ are the solitons that emerge from $u(x, 0)$. There also exists an oscillatory state (corresponding to the continuous spectum). For early times, the nature of the latter was clarified in my numerical study [52].

During this period and unknown to the Princeton–Bell Labs group, M. Toda found a *lattice* system [53] which supported solitary and periodic waves. The interaction potential has the form

$$V = (a/b)\, e^{-br_n} + ar_n + \text{const}, \qquad (ab) > 0, \tag{48}$$

and the equations of motion in dimensionless form can be written as

$$\ddot{r}_n = -[e^{-r_{n+1}} - 2e^{-r_n} + e^{-r_{n-1}}], \tag{49}$$

or

$$\ddot{Q}_n = \exp[-Q_n + Q_{n-1}] - \exp[-Q_{n+1} + Q_n], \tag{50}$$

or

$$\ddot{s}_n/(1 + \dot{s}_n) = s_{n+1} - 2s_n + s_{n-1}, \tag{51}$$

with

$$\dot{s}_n = e^{-r_n} - 1 \qquad \text{and} \qquad \dot{Q}_n = s_n - s_{n+1}. \tag{52}$$

He also displayed a soliton solution (48)

$$e^{-r_n} - 1 = \beta^2 \sec^2(\alpha n \mp \beta t), \qquad \beta = \sinh \alpha.$$

As Toda indicates and Ford confirms [54], the above developments were stimulated by the numerical results of Ford and Waters [55]. In 1968, when I attended the International Conference on Statistical Mechanics in Kyoto, he showed me formal analytic calculations of a two-soliton interaction [56]. I was amazed because of my "intuitive" belief in the difficulty of treating *discrete* nonlinear systems and because he could treat the interaction of left- and right-going nonlinear waves. (See my comment at the end of [56].)

A numerical simulation by Saito *et al.* [57] seemed to suggest soliton decay on the Toda lattice. J. Ford, one of the contributors to energy sharing problems of cubic and quartic lattices [55], remarked [58],

> ... everyone including me thought that the Toda lattice was non-integrable. Thus, as we began the studies described in the enclosed [59] we were convinced we were going to observe non-inegrable behavior (i.e. soliton decay). Indeed, we were so certain of this that we were performing the study only as a preliminary to studies of the Toda lattice with unequal masses. Then much to our surprise every test we ran indicated integrability. Eventually, we became convinced of integrability and sent the enclosed off to *Prog. Theor. Phys.* [59]. At the same time, we sent preprints to Henon [60], among others. Then, my God, by return of mail, we received the complete set of integrals for the Toda lattice from Henon. He noticed that one could easily get the Toda integrals (constants of the motion) directly from the integrals of the hard point gas. Within a day or so of receiving the complete set of integrals from Henon, Herman Flaschka [61] passed through Atlanta.... When I advised him of the recent happenings, Herman reached into his briefcase and pulled out his recent calculations on the Toda lattice using a version of inverse scattering that he had just developed. Within a few hours, he calculated the Henon integrals using inverse scattering theory. [The reference insertions are mine.]

Remark 5. *Sine–Gordon result.* Fermi, Heisenberg, Ulam, and others pointed out that field theories for elementary particles could be nonlinear. Perring and Skyrme [62] studied what is presently called the "sine–Gordon" equation

$$q_{xx} - c^{-2} q_{tt} = \kappa^2 \sin q, \tag{53}$$

as a model for a nonlinear meson field theory. The equation has been known in differential geometry since the end of the last century [63] and first arose in modern times as a model for the one-dimensional movement of dislocations in solids [64, 65]. Equation (53) is Lorentz invariant and can be transformed to "light-cone" or characteristic coordinates, or

$$\partial_{\xi\eta} q = \kappa^2 \sin q. \tag{54}$$

Perring and Skyrme found stationary solutions in a frame of reference moving with velocity v, or if $s = (x - vt)/(1 - v^2)$ then (53) with $c = \kappa = 1$ becomes

$$d^2\alpha/ds^2 = \sin\alpha, \tag{55}$$

and solutions are

$$\sin(\tfrac{1}{2}\alpha) = \pm k\,\mathrm{sn}[(i(s - s_0); k)], \qquad v > 1, \tag{56}$$

$$= \pm\mathrm{cn}[k^{-1}(s - s_0); k], \qquad v < 1 \tag{57a}$$

or

$$\alpha = 4\tan^{-1}\{\exp[\pm(s - s_0)]\}, \qquad v < 1, \tag{57b}$$

where sn and cn are the Jacobi elliptic functions and $0 < k < 1$. The $(\pm)$ signs in (57b) refer to solutions that are commonly called particles, kinks, or fluxons $(+)$ or antiparticles, antikinks, or antifluxons $(-)$, respectively.

In the synergetic mode, they computed numerically two-"particle" interactions by having one particle approach the boundary $x = 0$ where $q(0, t) = 0$ was imposed. To their "surprise" they found elastic scattering and then sought and found the corresponding nonlinear solution for particle–particle collision,

$$\tan(\alpha/4) = v\sinh[x/(1 - v^2)^{1/2}]/\cosh[vt/(1 - v^2)^{1/2}], \tag{58}$$

and for a particle–antiparticle collision,

$$\tan(\alpha/4) = v^{-1}\sinh[vt/(1 - v^2)^{1/2}]/\cosh[x/(1 - v^2)^{1/2}]. \tag{59}$$

No further work came from this computational probe.

Why was this pioneering salient lost? One possibility is that the majority of elementary particle physicists, at that time, believed in linear field theories. Furthermore, they felt that there was little insight to be gained from one-space dimensional problems. Another, more probable, explanation is that the computational ambiance was neither broad nor *valued*. Nor was the simulation data base invested with structure that is required to sustain creative momentum to overcome the barriers of "establishment" intuition. In the third period, Makhankov and colleagues, Bialynicki-Birula and colleagues, and Simonov and Tjon are using the computer to study two- and three-space dimensional problems relevant to elementary particle physics (as described in Section 4.4).

Remark 6. *Numerical algorithms.* The nonlinear lattice results were obtained with the simple centered time-dependent algorithm (8). The initial studies of the KdV and mKdV equations were made with a centered 3-level (explicit) leap-frog algorithm, as described in Appendix A for the mKdV equation. These were designed to conserve $\sum_n u(n\,\Delta t, t)$ at alternate time levels and to conserve $\sum_n u^2(n\,\Delta x, t)$ in the

limit ("semi-continuous") where time derivatives are considered exact. No scheme was found to conserve the discretized version of $T^{(3)}$ in (34).

Our algorithm gave stable results for the two-soliton interaction studies, but developed a typical leap-frog instability prior to $\frac{1}{2}t_R$ or t_R for the evolution of sine-wave initial conditions. Kruskal and I overcame this with a dissipative restart procedure. That is, we obtained restart waveforms at levels $n+1$ and n from averaged data at levels $(n+2, n+1, n)$ and levels $(n+1, n, n-1)$, respectively. For the run in the movie we did this just before $\frac{1}{2}t_R$ but *not* before t_R, and so were able to see a spatially localized "flicker" develop that seems to be an indicator of a developing nonlinear instability. This four-level filtering process is equivalent to introducing dissipation for a small time interval and may account for the somewhat smoother near-recurrence waveform that we observed as compared to the results of Abe and Inoue [66], obtained by *spectral* methods.

Many algorithms have since been developed. Some are discussed by Eilbeck in a thorough and balanced review [67]. Recently, Fornberg and Whitham [68] gave an account of the application of a robust and accurate *pseudospectral* method to the generalized KdV equations

$$u_t + u^p u_x + u_{xxx} = 0 \qquad (p = 1, 2, 3, \text{ and } 4), \tag{60}$$

and to

$$u_t + uu_x + \int K(x-\xi)\, u_\xi \, d\xi, \qquad K = (\nu/2)\, e^{-\nu|x|}, \tag{61}$$

and other equations *all* with periodic boundary conditions. Their paper is a balanced blend of asymptotic and stability analyses and computer simulations with parameters chosen to illustrate numerous interesting effects. The paper is brightened with good oblique-projective graphs of waveforms and summary graphs. Appendix B contains a good discussion of numerical instabilities (they also observed the temporal leap-frog instability discussed above) and aliasing in pseudospectral algorithms.

As with pioneering experiments in physics using rudimentary apparatus, the early algorithms provided high-quality detailed information which stimulated insights for analytical progress. However, the next steps will require more accurate and more efficient algorithms. An illustration is the recent works of Ablowitz, Kruskal, and Ladik [69], Bogolubskii and co-workers [70], Bona, Pritchard and Scott [71], Santarelli [72], and Lewis and Tjon [73], who examined the interaction of two solitary waves for systems that are presently known to be nonintegrable (namely, ones that do not have an infinity of conservation laws). The last three groups studied the "regularized" long-wave RLW equation

$$u_t + u_x + uu_x - u_{xxt} = 0, \tag{62}$$

which has the solitary-wave solution

$$u = A\,\mathrm{sech}^2[(x-ct)/\Delta], \qquad \Delta = [(4A+6)/A]^{1/2}, \qquad c = 1 + 2A/3. \tag{63}$$

Bona *et al.* found an oscillatory state was left behind whose maximum amplitude (over several runs) was about 1.1% of the smaller (overtaken) solitary wave in a head-to-tail interaction. Santarelli and Lewis and Tjon chose amplitudes $A_1 > 0$ and $A_2 < -(3/2)$ so that $c_1 > 0$, $c_2 < 0$ and the solitary waves were head-on. The inelastic effect was much greater and *additional* solitary entities appeared.

Remark 7. *Graphics.* As our analytical insight matured, the character of the graphical representation became focussed on particular phenomena. FPU plotted waveforms $y_n(t)$ and modal energies as shown in Fig. 2. When it became clear that progressive waves with boundary periodic conditions contained the same effect, we began tracking trajectories of waveform extrema; this proved informative, for it allowed us to see phase shifts arising from localized entity interactions.

This "Riemann-invariant" filtering was applied to a cubic lattice with periodic boundary conditions that was strongly excited with a low-mode progressive wave. That is, if a *discrete* approximation to the Riemann invariant is

$$\tilde{r}_{\pm}(n, t) = \tfrac{1}{2}\{\pm \dot{y}_n + \tfrac{1}{3}(N/\alpha)[(1 + 2\alpha(y_{n+1} - y_n))^{3/2} - 1]\} \qquad (1 \leqslant n \leqslant 2N),$$

then I chose

$$y_n(0) = a \sin(\pi n/N) \qquad (1 \leqslant n \leqslant 2N)$$

and

$$\dot{y}_n(0)$$

so that

$$\tilde{r}_+(0) = 0.$$

This smooth initial condition with $a = 10.132$ ($\approx \pi^2$), $\alpha = 1$, and $= 100$ evolved to breakdown at one-half a linear period ($t_B/t_L = \frac{1}{2}$) and formed about 46 "localized" entities each about four lattice-intervals wide, as shown in Fig. 8. The trajectories of $\max_n \tilde{r}_-(n, t)$ were tracked and the velocity–amplitude diagram of Fig. 9 was determined. The recurrence time was estimated on the basis of the location the maxima of the prime-numbered modes. However, at t/t_L slightly greater than 5.5, the solution became singular and the computation ceased. Apparently, this resulted from an interaction that caused one particle to exceed the confining potential energy of a cubic lattice as described in Eq. (6) above. Recently, Ferguson *et al.* [75] developed a perturbation method using action variables of the Toda lattice as basis functions for strong nonlinear excitations of the cubic lattice; their method is "... partly rigorous, partly heuristic... ." However, for the duration of the simulation just described, they identify 19 of the 46 localized entities as analogs of Toda-lattice solitons and the remaining entities as "... near-linear wave packets."

The oblique projections of $\psi(x, t)$ developed by the Manchester group (Bullough, Eilbeck, Caudrey) have provided useful and artistically pleasing global summaries of

RUN 68-20, $t_B/t_a = 1/2$

	t/t_a	MAX $\tilde{r}_-$ x	MAX $\lvert\tilde{r}_+\rvert$ x	TOTAL ENERGY
A	0	36.45	0	1009.54
B	1/2	36.46	7.77	1009.55
C	2.0	70.83	18.47	1009.77
D	5.5	70.72	19.16	1010.20

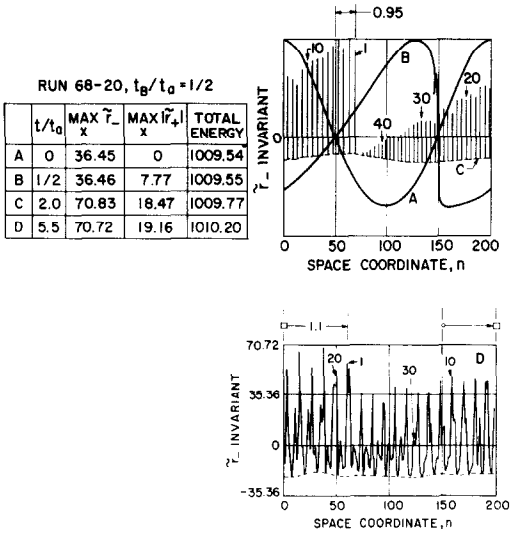


FIG. 8. Riemann-invariant filtered waveforms $\tilde{r}_-(n, t)$ for a cubic lattice with an initial strong progressive wave excitation that causes breakdown in one-half a linear period, curve B.

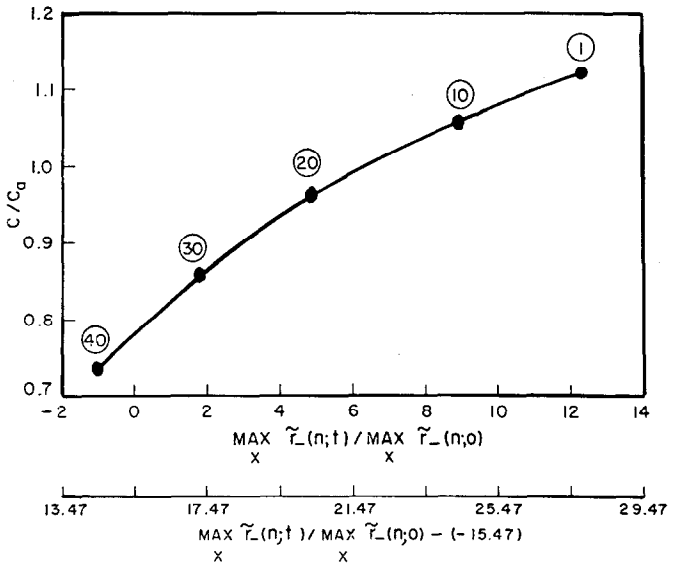


FIG. 9. Lattice solitary-wave speed vs amplitude diagram. Note that the smallest pulses are travelling at the linear group velocity.

nonlinear wave phenomena. For example, Fig. 10 gives $\psi(x, t)$ for the interaction of two solitons of the nonlinear Schrödinger equation (79). The phase shift of the right-going soliton is evident. Figure 11 shows $\psi(r, t)$, solutions of the cylindrically symmetric sine–Gordon equation with a localized impurity current $j(r)$,

$$\psi_{rr} + r^{-1}\psi_r - \psi_{tt} - j(r) \sin \psi = 0, \tag{64}$$

where

$$j(r) = 1 + a \operatorname{sech}^2(r - R_1).$$

Exhibited are nearly two periods of a *permanent* oscillation of a cylindrically symmetric "pulson." The pulson "falls" toward the origin and is reflected by the localized impurity current at R_1. If one adds a damping term, the oscillation decays. However, if one switches on a constant bias (that is, a constant is added to the right side of (64)) for an appropriate time interval a tunable periodic oscillation is obtained [76]. The collapse time of analogous moving entities was first studied numerically by Bogolyubsky and Makhankov [77]. They investigated the three-dimensional nonlinear Klein–Gordon equation (ϕ^4), excited initially with a radially symmetric solitary wave solution. Cylindrically symmetric studies of the sine–Gordon equation were indicated by Makhankov [78, Sect. 7.3] and described in detail by Christiansen and Olsen [79]. Figure 12 shows $\sin(\frac{1}{2}\psi(x, y))$ at various t [80]. Here ψ is the solution of the full two-dimensional sine–Gordon equation with boundary conditions that simulate an interaction between expanding ring and anti-ring "solitons" (or pulsons). The initial condition (not shown) is a circular ring-soliton. We see the ring soliton moving outward and reflected by the anti-ring soliton (the boundaries $x = \text{const.}$) and emitting radiation.

The use of color and cinema can greatly enhance the perception of small unexpected phenomena. They also provide other "parameters" to aid the retention process. This enhances the mind's ability to recall and correlate old and new results. Figs. 13a and b contain black and white renditions of color photographs provided by S. T. Zalesak and S. L. Ossakow. (Unfortunately, the economics of publishing require this compromise.) The two frames at $t = 0$ and $t = 1300$ show the unstable evolution of a small perturbation in the ion density at the bottom of the ionosphere into a rising low-density plasma "bubble" [81]. These are finite-difference solutions of

$$\begin{gathered} \partial_t n + \partial_x(nu) + \partial_y(nv) = -\nu_R n, \\ \nabla \cdot (\nu_{in} n \nabla \phi) = -\bar{\nu}_{in} E_0 \partial_x n \qquad \text{and} \qquad (u, v) = (c/B_0)(-\partial_y \phi, \partial_x \phi), \end{gathered} \tag{65}$$

where the variables n, ϕ, u, v, are functions of x, y, and t; ν_R and ν_{in} are prescribed functions of y; and $\bar{\nu}_{in}$, E_0, c, and B_0 are constants. We see small electron-density regions (blue = B and turquoise = T) have been convected up into the large electron density (red = R) region, a small effect difficult to observe in black and white *contour* plots, e.g., Fig. 13c at $t = 1364$.

Easy-to-use computer languages are being developed that will aid in producing

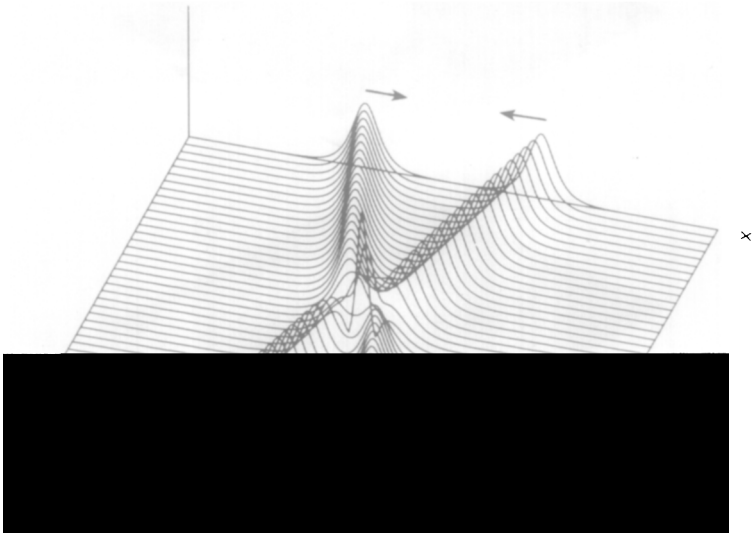


FIG. 10. Oblique projections $\psi(x, t)$ of two-soliton interactions. Solutions of the nonlinear Schrödinger equation $i\psi_t + \psi_{xx} + \kappa\psi\,|\,\psi\,|^2 = 0$ with initial conditions $\psi(x, 0) = 1.5[\text{sech}(1.5(x-10)\,e^{(0.375(x-15))} + \text{sech}(1.5(x-20))\,e^{-i(0.375(x-15))}]$, and with boundary conditions $\psi(0, t) = \psi(30, t) = 0,\ 0 \leqslant x \leqslant 30,\ 0 \leqslant t \leqslant 25$.

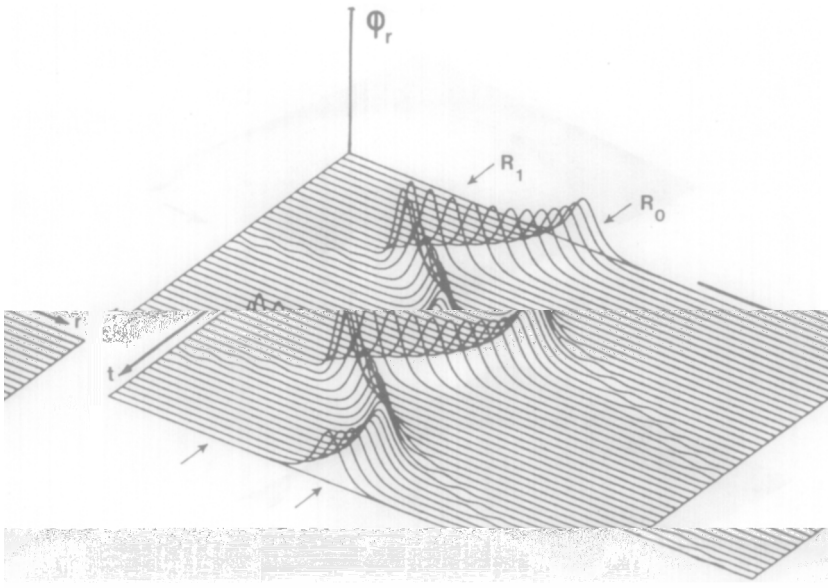


FIG. 11. Solutions $\psi_r(r, t)$ of azimuthally symmetric sine–Gordon equation with a current impurity $j(r)$, $\psi_{rr} + r^{-1}\psi_r - \psi_{tt} - j(r)\sin\psi = 0$. Exhibited are permanent oscillations of a pulson which has a "ballistic" behavior. It "falls" into the origin and is reflected by the localized impurity current at R_1.

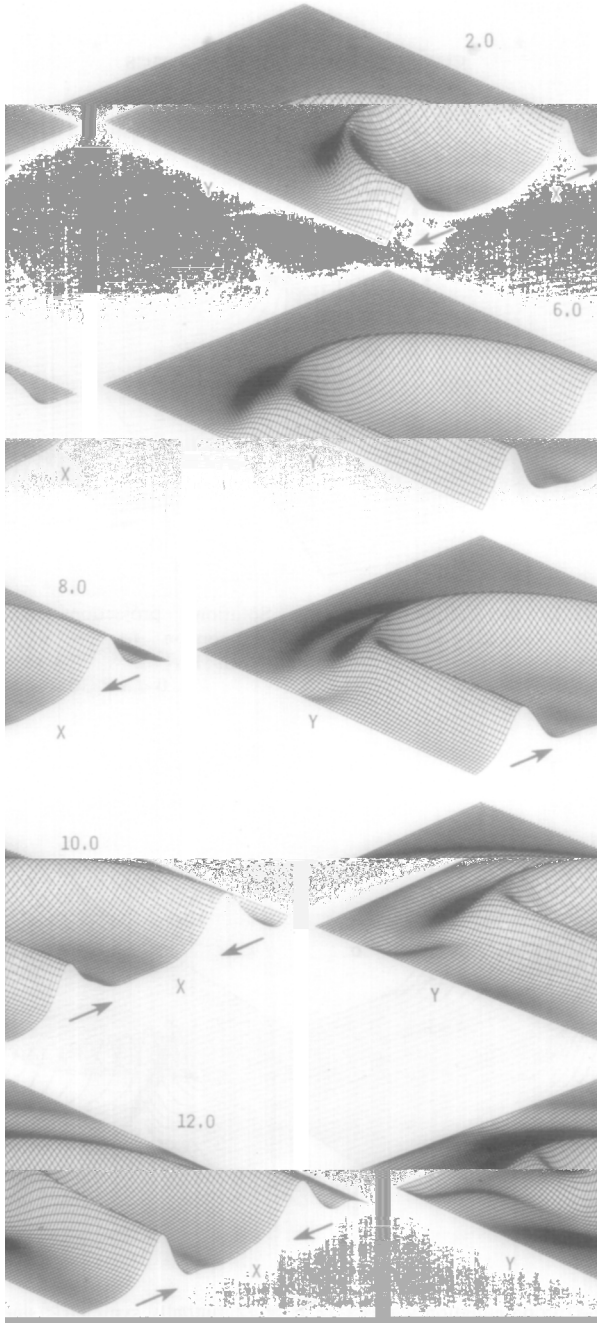


FIG. 12. Interaction of a "ring" pulson with near boundaries. $\sin(\frac{1}{2}\psi(x, y))$ vs (x, y) at $t = 2.0$, 6.0, 8.0, 10.0, 10.0, 12.0 for $\psi_{xx} + \psi_{yy} - \psi_{tt} = \sin\psi$, with initial conditions: $\psi(x, y, 0) = 4\tan^{-1}\exp[4 - (\{(x+3)^2 + (y+7)^2\}^{1/2})/0.436]$; $\psi_t(x, y, 0) = 4.13\ \mathrm{sech}[4 - (\{(x+3)^2 + (y+7)^2\}^{1/2})/0.436]$ $(-10 \leqslant x \leqslant 10$ and $-7 \leqslant y \leqslant 7)$; and boundary conditions: normal derivative $= 0$ on boundaries $x = 10$, $y = 7$, $y = -7$ and $\psi_t(-10, y, t) = 0$. This figure was provided by P. Lomdahl and P. Christiansen.

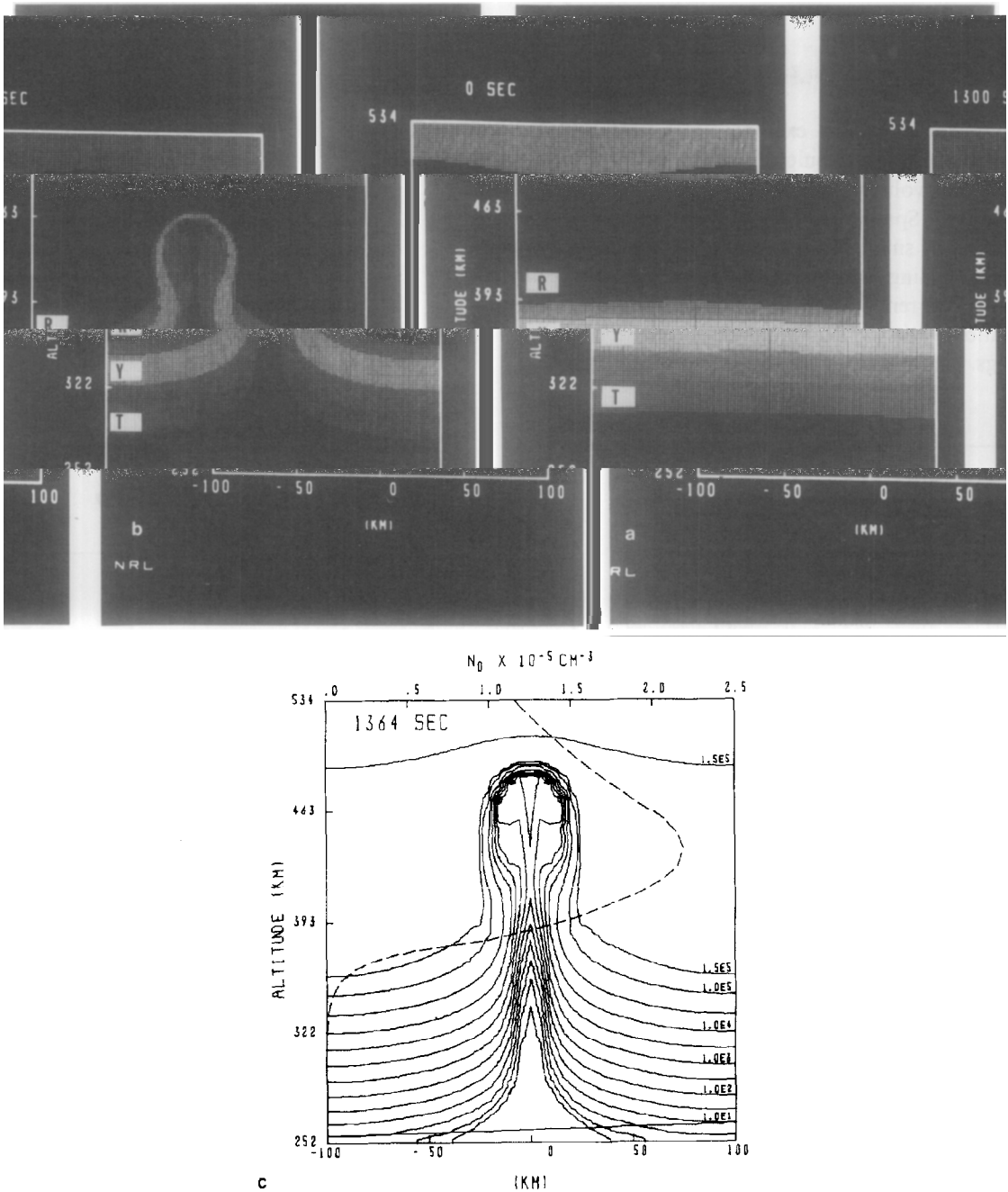


FIG. 13. Evolution of small localized perturbation in the lower ionosphere at $t = 0$ (13a) into a rising plasma "bubble" at $t = 1300$ (13b). The horizontal scale (x) is east-west with the observer looking southward. The color code of the ion density $n(x, y)$ is: R = red $(1.5 \times 10^5 - 2.5 \times 10^5)$ and orange $(1.0 \times 10^5 - 1.5 \times 10^5)$; Y = yellow $(1.0 \times 10^4 - 1.0 \times 10^5)$ and green $(1.0 \times 10^3 - 1.0 \times 10^4)$; T = turquoise $1.0 \times 10^2 - 1.0 \times 10^3$) and blue $(0 - 1.0 \times 10^2)$. Figure (13c) gives contour representation of $n(x, y)$ at $t = 1364$ which is to be compared with Fig. (13b) at $t = 1300$. This figure was provided by S. T. Zalesak and S. L. Ossakow.

cogent still graphics and cine-films, for example [82]. It would be desirable for problems of waves and fluctuating or turbulent fluids to develop robust algorithms to track and plot *extremal* lines, areas and volumes in one, two, and three dimensions. These diagrams will probably be "noisy." Spatial and temporal correlations should be used to obtain histories of the location of small but important regions when they are hidden in a busy background. Color, shading, and alternate view angles will facilitate the recognition of these event. A current example is obtained from Siggia's simulations of the 3D Navier–Stokes equations with periodic boundary conditions at a Reynolds number, Re = 100 [83]. In Figs. 14a and b we see two views of the same

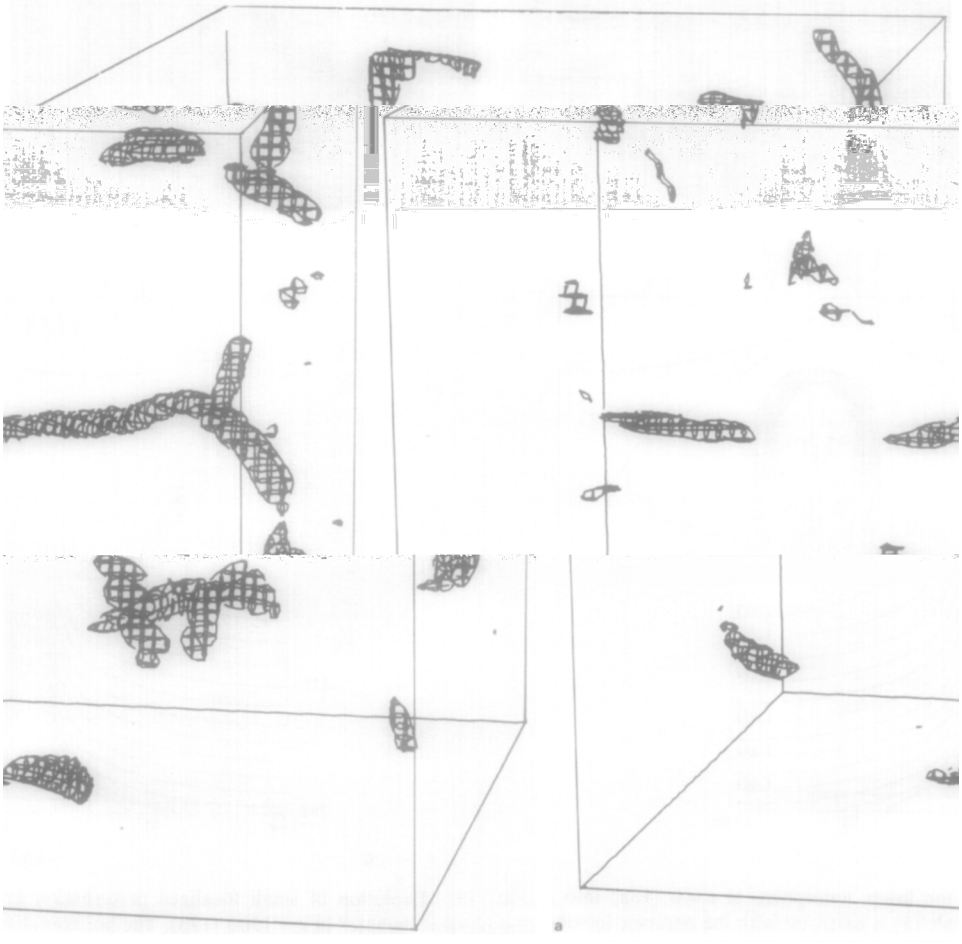


FIG. 14. Alternate views of regions of mean-square vorticity excess in a 3D simulation of the Navier–Stokes equation at Re = 100 with periodic boundary conditions. The views in Fig. (a) and Fig. (b) are both from the first quadrant. This figure was provided by E. Siggia.

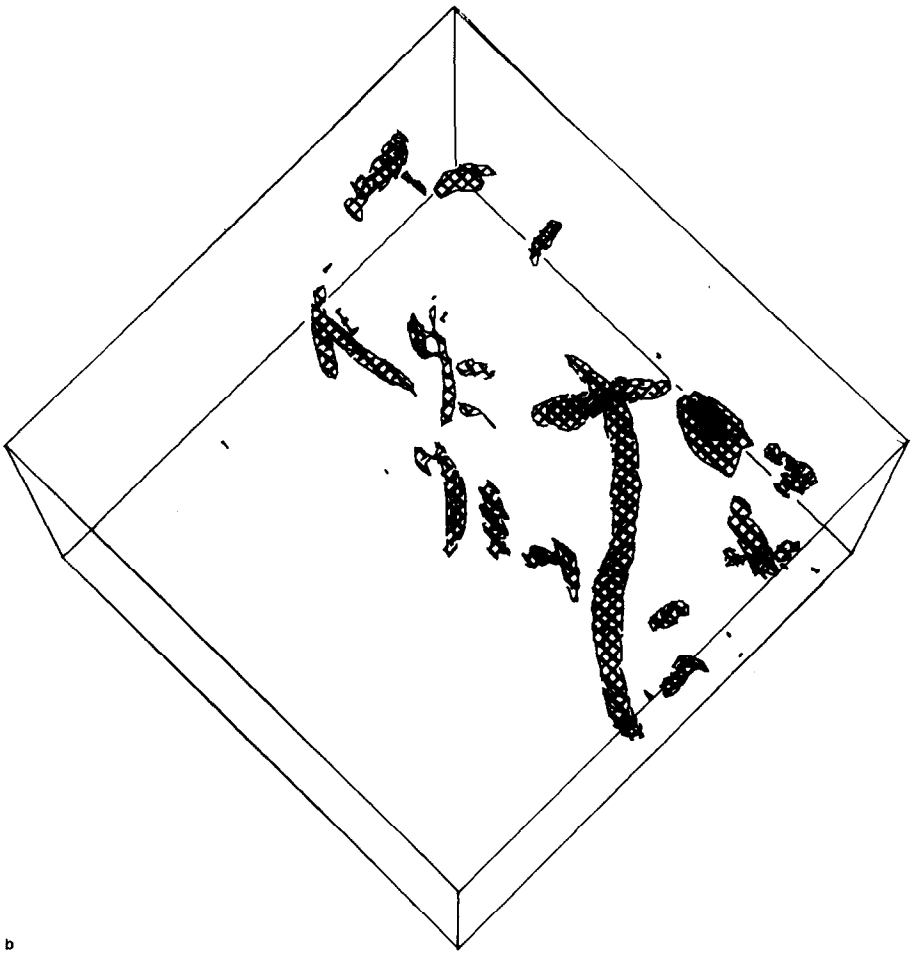


FIG. 14—*Continued.*

periodic box. The shading covers regions where the mean-square vorticity exceeds a prescribed magnitude. Changes in this magnitude do not change the qualitative appearance of the vortex tube. These tubes are believed to be generated by a balance between vortex stretching and viscous diffusion. ▮

P. D. Lax, who was close to our analytical and computational milieu, took the first steps in the direction of mathematical generalization by introducing an operator notation [42]. He noted the invariant quantities $\int T^{(n)}\,dx$ and the invariant eigenvalues of

$$L = d^2/dx^2 + (u/6), \tag{66}$$

(for (28) with $\delta^2 = 1$). He asked how the potential $u(x, t)$ could be varied such that the eigenvalues of $L(t)$ remained invariant. For such a deformation, $L(t)$ must have a unitary equivalence

$$U^*(t)\, L(t)\, U(t) = L(0), \tag{67}$$

for the one-parameter family of unitary operators U, which have the property

$$U_t = BU, \tag{68}$$

where $B(t)$ is antisymmetric, or

$$B^* = -B. \tag{69}$$

Differentiating (67) and using (68) and (69) we obtain

$$L_t = BL - LB = [B, L],$$

where $L_t = u_t$ is a scalar operator. He observed that (69) has an infinite sequence of solutions $B_0, B_1, B_2, \ldots$, where B_q is a linear symmetric differential operator of order $2q + 1$, and

$$B_1 = -(d^3/dx^3) - u(d/dx) - \tfrac{1}{2}(du/dx), \tag{70}$$

satisfies $[B_1, L] = -\frac{1}{6}u_{xxx} - \frac{1}{6}uu_x$. If we substitute into (67) we obtain the KdV equation, hence proving that KdV flows leave the eigenvalue invariant. That is, if ϕ_0 is the eigenfunction of $L(0)$ and ϕ is the eigenfunction of $L(t)$

$$L(0)\, \phi_0 = \lambda \phi_0 \qquad \text{and} \qquad L\phi = \lambda \phi, \tag{71}$$

then, since

$$L(t)\, U(t)\, \phi_0 = \lambda U(t)\, \phi_0, \tag{72}$$

it follows that

$$\phi(t) = U(t)\, \phi_0 \qquad \text{and} \qquad \phi_t = B\phi. \tag{73}$$

For $B = B_1$, we obtain from (73)

$$\phi_t + 4\phi_{xxx} + u\phi_x + \tfrac{1}{2}u_x\phi = 0. \tag{74}$$

Since ϕ is the eigenfunction of L, or

$$\phi_{xx} + (\tfrac{1}{6}u - \lambda)\phi = 0, \tag{75}$$

we can differentiate with respect to x and substitute in (74) to obtain

$$\phi_t + (4\lambda + \tfrac{1}{3}u)\, \phi_x - \tfrac{1}{6}u_x\phi = 0, \tag{76}$$

a first-order linear partial differential equation, if u is prescribed. It can be studied by the method of characteristics, or

$$dx/dt = 4\lambda + \tfrac{1}{3}u \tag{77}$$

and

$$d\phi/dt = \tfrac{1}{6}u_x\phi \qquad \text{(along characteristics).}$$

Thus, the zeroes of ϕ propagate along characteristics.

Lax noted [84]: "In a film depicting the time evolution of an initially sinusoidal solution of the KdV equation, made by Gary Deem at Bell Laboratories under the direction of Kruskal and Zabusky, there are eight clearly distinguishable 'solitons', each pursuing its own path. It is tempting to try to relate the paths of these solitons to the characteristics... ." Thus he was on his way to solving the periodic KdV problem. Supporting analytical and numerical work was done by J. M. Hyman [85], who showed the *exact* recurrence of initial (nonsinusoidal) states. He also considered cases where a small high-frequency random perturbation was superimposed initially.

C. Gardner [86] recognized that the periodic KdV problem could be written as a *Hamiltonian* system and showed that if

$$I^{(m)} = \int T^{(m)}\, dx,$$

where the integration is over one period and $T^{(m)}$ are the conserved densities of the KdV equation discussed above, then

$$0 = dI^{(m)}/dt = \int \left[\frac{\delta I^{(m)}}{\delta u}\right]\left[\frac{\delta I^{(n)}}{\delta u}\right] dx \equiv \{I^{(m)}, I^{(n)}\}, \tag{78}$$

and $(\delta/\delta u)$ is the Fréchet derivative. The last Poisson bracket expresses the fact that the constants of motion are in involution, i.e., $\{I^{(m)}, I^{(n)}\} = 0$. Thus, the system constitutes a completely integrable infinite dimensional Hamiltonian system—a first example of this class. Fadeev and Zakharov [87], in a remarkable paper that heralded the entrance of Soviet mathematicians, showed independently the "symplectic' structure underlying the KdV equation. We now know this to be a property of all *integrable* system like the KdV, mKdV and sine–Gordon equations.

Hirota introduced his ingenious "direct" method to construct the N-soliton solutions of the KdV equation [88] and the sine–Gordon equation [89].

The panorama of possible equations that are exactly integrable was exposed by the breakthrough paper of Zakharov and Shabat [90]. They built on Lax's operator approach and introduced a generalized 2×2 *scattering* form to linearize exactly the nonlinear Schrödinger equations (NLSE)

$$i\psi_t + \psi_{xx} + \kappa|\psi|^2\psi = 0. \tag{79}$$

This equation was first derived for nonlinear optics, but has since been shown to be relevant to nonlinear deep-water waves and intermediate-wavelength nonlinear waves on lattices. In fact, it can be derived from the KdV equation in an intermediate-wave limit.

Remark 8. *Integrability, instability, "collapse," and ergodic behavior.* Equation (22) was called the Zabusky equation by Toda [39] and Kalantarov and Ladyzhenskaya [91]. However, in 1871, Boussinesq [92] obtained a similar equation (with $u = y_x$) from a small-but-finite amplitude long-wavelength asymptotical analysis of the shallow water-wave equations. These equations support left-and-right propagating waves and are integrable [91]. Despite the stability of solitons, Berryman [94] has shown that short-wavelength plane wave perturbations are unstable. This follows from the linear dispersion relation. This result implies that integrability does not guarantee linear stability of solitary waves. Furthermore, for a certain class of large amplitude initial conditions, the solution of (22) can become singular or "collapse" [91] in a finite time. This phenomenon was also observed in the cubic lattice [74], as described in Remark 7.

Note the near-recurrent solutions of the cubic and quartic lattice are *not* obtained for the lattice with the "piecewise-linear" force law, also studied by FPU. That is, since the force law is not analytic, the system exhibits a more ergodic behavior. ∎

3.3. *Generalization, Abstraction, and Application (1972–Present)*

After the exact linearization of the NLSE, analytical results came in a torrent. In Fig. 1 of their preface Lonngren and Scott [95] illustrated the exponential surge of papers that followed. In particular, Wadati [96] linearized the mKdV equation with the 2×2 scattering scheme; the Clarkson group (M. J. Ablowitz, D. J. Kaup, A. Newell, and H. Segur) built on the Zakharov and Shabat work and introduced a simple-and-powerful algebraic procedure that was applied to the sine–Gordon equation [97]. They emphasized that the method could be considered a nonlinear generalization of Fourier transform analysis for linear problems.

The analytical mode was now ascendant. Although the evergrowing mathematical literature is beautiful and remarkably diverse, it would not serve the computational thrust of the present paper to detail it here, Besides, Bullough and Caudrey [98] have given a presentation of these aspects. However, I wish to leave the reader with a feeling for this penetration into diverse classical areas of mathematics, including:

- Algebraic geometry: Multi-sheeted Riemann surfaces; Finite-zoned potentials; Abelian varieties and theta functions. (S. P. Novikov, V. E. Zakharov, L. Dikii, V. G. Drinfeld, B. D. Dubrovin, I. M. Gelfand, I. M. Krichever, V. B. Mateev, S. V. Manakov, Yu, I. Manin, H. P. McKean, P. van Moerbeke, E. Trubowitz, etc.)
- Differential geometry: Prolongation structures and Bäcklund transformations. (F. B. Estabrook, H. D. Wahlquist, R. Hermann, H. C. Morris, J. Corones, R. Sasaki, F. A. E. Pirani, D. C. Robinson, etc.)

Commuting operators and nonlinear evolution equations. (P. D. Lax, V. E. Zakharov, etc.)

Integral equations and inverse scattering (or isospectral transform theory). (M. J. Ablowitz, D. J. Kaup, A. C. Newell, H. Segur, M. Wadati, M. Toda, V. E. Zakharov, F. Calogero.)

Nonlinear ordinary differential equations and Painlevé transcendants. (N. T. Erugin, M. J. Ablowitz, A. Ramani, H. Segur, H. Flaschka, A. Newell, B. McCoy, C. Tracy, T. T. Wu, A. Fokas, M. Jimbo, T. Miwa, and M. Sato, etc).

Singular (pole) representation of nonsingular dynamical systems. (M. D. Kruskal, W. R. Thickstun, H. P. McKean, J. Moser, A. Airault, D. V. and G. D. Chudnovsky, F. Calogero, etc.)

Asymptotic methods for nonintegrable Hamiltonian systems. (V. I. Karpman and E. M. Maslov, V. V. Solov'ev, A. C. Scott, H. Flaschka, D. W. McLaughlin, A. L. Mason, etc.)

Although these developments were stimulated by basic questions in lattice dynamics, shallow water waves and magnetohydrodynamics, the application to optics, atomic physics, and Josephson junctions were soon realized by R. K. Bullough, P. J. Caudrey, J. C. Eilbeck and J. D. Gibbon, and A. C. Scott. Solid-state, condensed-matter, and elementary-particle physicists followed. Several papers that lucidly review this work include: S. Coleman [99], R. Jackiw [100], L. D. Fadeev and V. E. Korepin [101], and A. Luther [102].

4. New Directions

4.1. *Nonlinear Lattices*

The field of lattice dynamic with respect to solitons and heat transport has been thoroughly reviewed by Jackson [103]. See, in particular, K. Miura's 1973 work [104] on the cubic and quartic lattices and the Jackson, Pasta and Waters [104] on the cubic and quartic lattices and the Jackson, Pasta and Waters [105] study of the effect on energy transport of boundary layers adjacent to thermal "baths" in one-dimensional lattices. Part III of the film [41] shows the evolution of a cubic lattice, excited initially with a local "optical" excitation. Here alternate masses are displaced in opposite directions. For weak excitations, we see and immediate coupling to the long-wavelength branch which has been validated analytically [106]. For strong excitations, there is much more energy sharing among all the modes. However, new coherent propagating "entities" have arisen. These results have not been explained in an adequate analytical manner.

Studies of realistic lattice systems began with a two-dimensional Lennard-Jones model [107, 108]. An increase in thermal conductivity with increasing nonlinearity was found and an interpretation in terms of solitons was given [74]. Recent progress on strong nonlinear waves in realistic one- and two-dimensional systems is given in [109, 110].

Davydov in a series of papers and a review [111] has proposed a solitary entity as a carrier of band energy ("energy of valent vibration") in an α-helix protein molecule. One-dimensional lattice simulations by A. C. Scott and colleagues [112] have established a strong coupling between the acoustic and band-energy modes that has the appearance of a "lattice-soliton."

4.2. *Few-Mode Nonlinear Systems*

The behavior of nonlinear, iterative mappings and low-order differential equation systems *may* also contribute insight into the periodic, quasi-periodic and chaotic (or "turbulent") behavior of fluids, plasmas, biological ("population") systems, etc. In this brief section, I wish merely to illustrate again the impact of computation on the development of these diverse topics. The interested reader will find a guide through this fast-growing field in the recent reviews [R9, CG10].

Interest in iterative systems arose from possible "biological applications," etc. [113]. Work by N. Metropolis, M. L. Stein, and P. R. Stein [114] showed that as a parameter λ is varied, the qualitative behavior of iterates varies in a fashion independent of the particular function iterated. In particular, consider $x_{n+1} = F(x_n, \lambda)$ and specifically

$$x_{n+1} = \lambda x_n(1 - x_n) \qquad \text{and} \qquad x_{n+1} = \lambda \sin \pi x_n. \tag{80a, b}$$

For example, for a certain range of $\lambda < \lambda_1$ the iteration yields one fixed point. For $\lambda_1 < \lambda < \lambda_2$ one finds that the cycle is replaced by a cycle of double period, or

$$x_{n+2} = F(F(x_n))$$

has a fixed point. This period-doubling or bifurcation process continues until an infinite period and hence erratic behavior is attained [115]. These problems are ideally suited to computer studies which were guided in part by the analytic work of Ruelle, Smale, and others of the last 15 years.

Recently, M. Feigenbaum studied the period-doubling process. To elucidate his analysis he notes [116], "I numerically determined some parameters with an eye toward discerning some patterns. ... I immediately perceived the λ_n's were converging geometrically ... as n increased. This observation ... has never been made independently [and] was already a surprise." Since a convergence rate is a number invariant under smooth transformation he calculated

$$\delta_n = (\lambda_{n+1} - \lambda_n)/(\lambda_n - \lambda_{n-1}), \tag{81}$$

and found that it quickly approached $\delta = 4.6692...$. He continues [116] "I was reminded by P. Stein that period-doubling isn't a unique property of a quadratic map... . I decided to determine λ's in the transcendental case (84b) numerically ... and amazingly [found] the convergence rate was the same 4.6692... ." Thus, he discovered a "universal" theory which shows that qualitatively similar equations have identical quantitative behavior [117]. This concept of a period-doubling route to turbulence

[118] *seems* to have been substantiated in *some* laboratory experiments [119] and has engendered an explosive activity in analytical–computational synergetics. Feigenbaum notes [120], "the ... process of idea → computation → new idea → new computation → ... which I found amazingly stimulating in its rapid-fire unfolding, has seemed to me at the heart of a deeply significant method of performing theoretical research."

E. Lorenz, in the early sixties [121, 122], became interested in "numerical weather prediction" in order to clarify whether statistical (linear regression methods) could duplicate the performance of the "dynamical simulation method." He sought a system of equations which has *aperiodic* behavior and was sufficiently simple so that it could simulate a long stretch of weather with a reasonable amount of computation. He chose to represent a two-level model of the atmosphere, where thermal gradients produce instabilities, by a modal (orthogonal function) representation. He settled on a set of 12 ordinary differential equations whose solutions were [121]:

> unmistakably aperiodic ... the statistical forecasting method [was put] to test, and we found, incidentally, that it failed to reproduce the numerically generated weather data... .
>
> During our computations we decided to examine one of the solutions in greater detail, and we chose some intermediate conditions which had been typed out by the computer and typed them in as new initial conditions. Upon returning to the computer an hour later, after it has simulated about two months of weather, we found that it completely disagreed with the earlier solution. ... we soon realized that the two solutions did not originate from identical conditions. The computations had been carried internally to about six decimal places, but the typed output contained only three, so that the new initial conditions consisted of old conditions plus small perturbations. These perturbations were amplifying quasi-exponentially, doubling in about four simulated days, so that after two months the solutions were going their separate ways.
>
> It soon became evident that the instability of the system was the cause of its lack of periodicity. ... I immediately concluded that, if the real atmospheric equations behaved like the model, long-range forecasting of specific weather conditions would be impossible. ... The inevitable small errors in observing the current weather should therefore amplify and eventually dominate. ... Still, I felt that we could better appreciate the problems involved by studying a simpler example. ... The break came when I was visiting Dr. Barry Saltzman, ... he showed me some work on the thermal convection, in which he used a system of *seven* ordinary differential equations [123]. Most of his numerical solutions soon acquired periodic behavior, but one solution refused to settle down. Moreover, in this solution four of the variables appeared to approach zero.
>
> Presumably the equations governing the remaining *three* variables, with the terms containing the four variables eliminated, would also possess aperiodic solutions. Upon my return I put the three equations

$$dX/dt = -\sigma X + \sigma Y, \tag{82a}$$

$$dY/dt = -XZ + rX - Y, \tag{82b}$$

$$dZ/dt = XY - bZ. \tag{82c}$$

> on our computer and confirmed the aperiodicity which Saltzman had noted. We were finally in business.

The dependent variables X, Y, and Z measure the rate of convective overturning and

the horizontal and vertical temperature variations, respectively. The damping results from internal viscosity and conductivity and σ denotes the Prandtl number, while r is proportional to the Rayleigh number. These dissipative equations have a "strange attractor" for $r \geqslant r_c$,

$$r_c = \sigma(\sigma + b + 3)(\sigma - b - 1)^{-1},$$

and if $\sigma > b + 1$. The characteristic properties of these attractors and their relation to aperiodic solutions of forced disssipative systems is under active investigation for a variety of physical systems.

Remark 9. *Interactive, rapid turn-around computing.* From my observations and the above quotations, it is clear that interactive and rapid turn-around computing provides an opportunity to concentrate deeply and develop a special intuitive "feel" for the results. This noninterrupted mode augments the innovative process. This is easy to achieve for systems with a few dependent variables. A similar remark also applies to processing and visualizing the data base obtained from long-duration runs of large-scale simulations. ▮

4.3. *Multidimensional Nonlinear Continuous Systems*

In two or more space dimensions we have few analytical results for nonlinear evolution equations [124]. An exception is the Kadomtsev–Petviashvili (KP) equation [125]

$$\tfrac{3}{4}u_{yy} + (u_t + \tfrac{3}{2}uu_x + \tfrac{1}{4}u_{xxx})_x = 0, \tag{83}$$

which Satsuma [126] solved exactly for the oblique interaction of N solitons. Miles also analyzed the oblique interaction of two plane-wave solitons and has found regions of strong "resonant" behavior, which leads to unusual phase-shift behavior [127–129]. Yajima and colleagues have formulated an extended "Boussinesq-like" equation to describe plasma ion-acoustic waves [130] and have examined analytically and numerically the interation of two oblique soliton solutions [131].

Generally, one expects that most physically realistic multidimensional systems are nonintegrable. The computer must again be called on to provide heursitic results and validate perturbation methods. Even for integrable systems, where waveforms and numbers (e.g., recurrence times, resonant frequencies, number of waveform extrema) are required or where data from many different cases must be compared or processed, the computer is required. For example, the oblique projections of the waveform in [131] are a memorable summary of some of the resonant and near-recurrent processes.

F. D. Tappert [132] has studied the interaction of azimuthally symmetric *localized* states with various impact parameters as solutions of the NLSE

$$0 = i\psi_t + (\psi_{xx} + \psi_{yy}) + f, \tag{84}$$

where

$$f = \alpha^{-1}\psi(1 - \exp[-\alpha|\psi|^2]). \tag{85}$$

Equation (84) models self-focussing and filamentation of a laser beam in a nonlinear dielectric, where ponderomotive forces have been included. Tappert's movies summarize a wealth of information. Konno and Suzuki [133] study the evolution of a single beam with a nonsaturable and a different saturable nonlinearity, namely,

$$f \propto |\psi|^2 \qquad \text{and} \qquad f \propto \psi|\psi|^2/[1 + \alpha^2|\psi|^2]. \tag{86}$$

Bialynicki-Birula and his colleagues have been studying the 2D nonlinear Schrödinger equations with a logarithmic potential [134]. Makhankov and his group at Dubna have studied the interaction of "Q-solitons" [135, 136, R9] for

$$0 = \psi_{tt} - (\psi_{xx} + \psi_{yy}) + \psi - \psi|\psi|^2/[1 + |\psi|^2]. \tag{87}$$

To obtain the Q-soliton shape ϕ they take $\psi = \phi(r)\, e^{i\mu t}$ and solve the resulting nonlinear boudary value problem. The simulations are head-on collisions of Q-solitons with equal and opposite speeds (varying with μ) and *zero* impact parameter so that symmetry can be used to reduce the computer load by a factor of 4. They observe: "elastic (undistorted through passage) and weak inelastic collisions; decay of interacted states; decay through a resonance; and the creation of bound states." Similar behavior was found by Simonov and Tjon [R11].

P. L. Christiansen and P. Lomdahl [80] have been studying the collapse of elliptical "ring solitons" and interaction of circular "ring solitons" with different boundary conditions (Fig. 12). These are solutions of the 2D sine–Gordon equation

$$0 = \psi_{xx} + \psi_{yy} - \psi_{tt} - \sin\psi. \tag{88}$$

At Pittsburgh, we have been studying the interaction of localized dipolar vortex solutions of the incompressible Euler equations in 2D

$$\zeta_t + \zeta_x\psi_y - \zeta_y\psi_x = 0, \qquad \psi_{xx} + \psi_{yy} = -\zeta. \tag{89}$$

These, so-called translating "V-states" [137] are *piecewise-constant* regions of vorticity, $\bar{\zeta}_i$, which travel at a uniform U related to their circulation (or area). Their shapes can be solving the free-boundary nonlinear integral equation [138, 139]

$$\psi(x, y) + Ux = c_i, \qquad (x, y) \in \Gamma_i, \qquad i = 1, 2, \tag{90}$$

where

$$\psi = -(2\pi)^{-1} \sum_i \bar{\zeta}_i \int_{D_i} G(x - \xi, y - \eta)\, d\xi d\eta, \tag{91}$$

D_i is the domain within Γ_i, and

$$G = \tfrac{1}{2}\log[(x-\xi)^2 + (y-\eta)^2]. \tag{92}$$

Using the method of "contour dynamics" [140, 141], A. Schwartz has studied the zero impact-parameter interaction of a single V-state with a pair of oppositely signed point vortices indicated by the filled small circle. Figure 15 shows four "head-on" interactions. Only the upper half of the x–y plane is shown because of symmetry and in each panel time increases upward. All runs begin at $t = 0$ with the same V-state. The arrows in the lowest and highest panels show the direction of approach and separation of the nearby vortex states. Figures 15a and b show weak interactions with large and small phase shifts, respectively. In both cases the contour is left "ringing"; that is, the perimeter-deviation plots $[P(t) - P(0)]/P(0)$ vs t (where $P(t) = \oint ds$) show characteristic boundary oscillations. Figures 15c and d show strong "breaking" or

Contour dynamics was used by E. A. Overman, II and the author to study the head-on zero impact-parameter interaction of two V-states with the same circulation

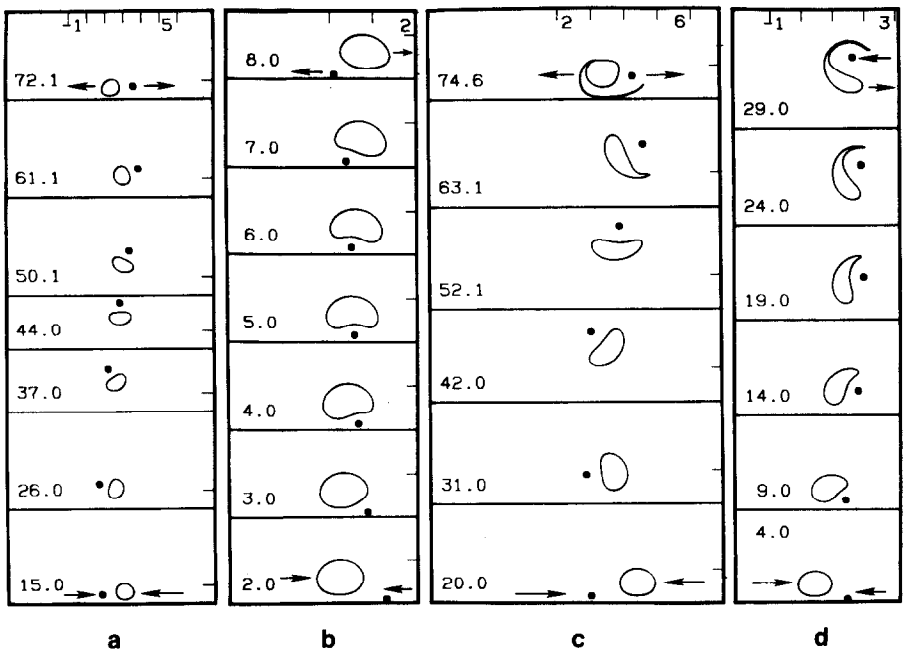


FIG. 15. Examples of the zero-impact parameter head-on interaction of a travelling dipolar V-state and a pair of point vortices. Solutions of the Euler equations in two dimensions. (a) Weak interaction with large phase shift. (b) Weak interaction with small phase shift. (c) Strong (breaking) interaction. (d) Strong (breaking) interaction. (Only the upper half of the plane is shown. The lower is obtained by symmetry.) In panels (a) and (c), the V-state approaches from the right and in panels (b) and (d) it approaches from the left. This figure was provided by A. Schwartz.

but different areas and different axis-offset distances. In Fig. 16, we see the upper-half plane contours for $t = 0$ and $t = 60$ with the trajectory of the center of areas given as a dashed time. This interaction suggests that translating V-states need not be symmetric. We also show a typical diagnostic at $t = 0$, namely, curvature vs arc length, which aids in elucidating fine-scale phenomena and assessing the numerical quality of the runs, particularly when breaking takes place [142].

Makino, Kamimura, and Taniuti [143] and McWilliams and Zabusky [144] have been studying the interaction of "modon" solutions of the quasigeostrophic equivalent-barotropic equations

$$\begin{aligned} \zeta_t + \zeta_x \psi_y - \zeta_y \psi_x &= -\beta \psi_x, \\ \psi_{xx} + \psi_{yy} + \gamma^2 \psi &= -\zeta. \end{aligned} \tag{93}$$

These modons [145] are localized stationary states that translate uniformly with velocity c and are of interest in gradient-drift plasmas [143] and atmospheric "blocking" phenomena [145]. We have studied those with vorticity distribution ζ

$$\zeta = -cq^2 \sin\theta \begin{cases} J_1(kr)/J_1(k), & r < 1, \\ K_1(qr)/K_1(q), & r > 1, \end{cases} \tag{94}$$

where the structure parameters k and q and the speed c satisfy the relations [143]

$$q^2 = (\beta/c) + \gamma^2 \qquad \text{and} \qquad [k^{-1}J_2(k)/J_1(k)] = [q^{-1}K_2(q)/K_1(q)]. \tag{95}$$

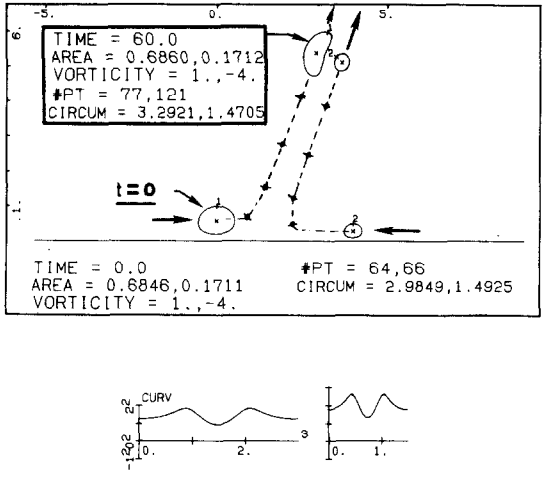


FIG. 16. Contour simulation of the interaction of two approaching (head-on) translating V-states with the same circulation. The upper panel shows the contours in the upper-half plane at $t = 0$ (below) and $t = 60$ (above) and the trajectories (dashed lines) of the center of areas. Tic marks indicate intervals, $\Delta t = 12.0$. The curvature $\kappa(s, 0)$ is plotted for each contour. This figure was provided by E. A. Overman, II.

The J_n are the Bessel functions of the first kind and the K_n are the modified Bessel functions of the second kind. Figure 16 shows a sequence of frames (time increases downward) of a zero-impact parameter head-to-tail interaction between modons, initially translating to the left at $c_1 = -0.75$ and $c_2 = -1.75$. (They are viewed in a frame of reference with velocity $= -1.25$ so in frame a they are approaching.) Here $\beta = 1$, $\gamma^2 = 2.0$, $q_1 = 0.8165$, $k_1 = 3.897$, $q_2 = 1.195$, $k_2 = 3.951$. Note after a strong interaction in which the slower modon (No. 1) is "dragged around" the faster modon (No. 2), we see a reformation into *two* solitary eddy states and two very small elongated vortex regions. Note, in frame e, modon No. 1 is reduced in size from its initial size. In a careful examination of the trajectories of the vorticity maxima, we find a speed change due mainly to vorticity rearrangement. It is possible to find parameters that yield modon configurations which minimize this speed change. Thus, the interactions are soliton-like; that is the vorticity maxima experience a phase shift and there is a very small excitation of internal degrees of freedom. However, for other parameters, new "inelastic" effects are observed, including: vorticity filamentation following moderate-to-strong interaction; modon "capture" (component monopoles of the same sign merge) in the overtaking (head-to-tail) mode; and the fission of modons into their component monopoles in the head-on mode.

4.4. *Analytical–Computational–Experimental Comparisons*

In closing, let us touch briefly on the relation of all the above to experiment. Progress in our understanding of the natural sciences has always depended upon the give-and-take between modeling (or theorizing), analysis, and experiment. With large-scale computers, we can process experimental data from a variety of sensors and juxtapose them readily with large-scale simulations—numerical solutions of ordinary and partial differential equations, etc. The insights gained from attempting to bring these results into agreement can synergize the rate of improvement of models, algorithms, analytical methods, and experimental procedures. The environment of shallow water waves is a splendid domain for examining this mode of working and the recent paper by Bona, Pritchard, and Scott [146] (discussed below) illustrates it.

In the laboratory experiment, a wavemaker at one end of a long tank generates small-but-finite amplitude waves which are sampled continuously at spatial intervals downstream, before the leading perturbation is reflected from a nearly obsorbing beach. Zabusky and Galvin [147] used a continuous sinusoidal wavemaker and were the first to examine features of the data that were a property of the KdV equation. They did this for Ursell (UR) or Stokes (S) numbers

$$Ur = S = 4/9\delta_0^2 = a\lambda^2/d^3$$

up to 153.4, where d is the still water depth, λ is the wavelength and a is the amplitude of the perturbation. (Note, in [147], experiments with three different Ursell numbers were performed, namely: 21.9, 95.1, and 153.4. Unfortunately, misprints caused them to be given as 21.95, 48.16 and 777 in entry 16 of Table 1. However, the correct values of δ_0^2 are given in Table 1.) They made several assumptions to relate

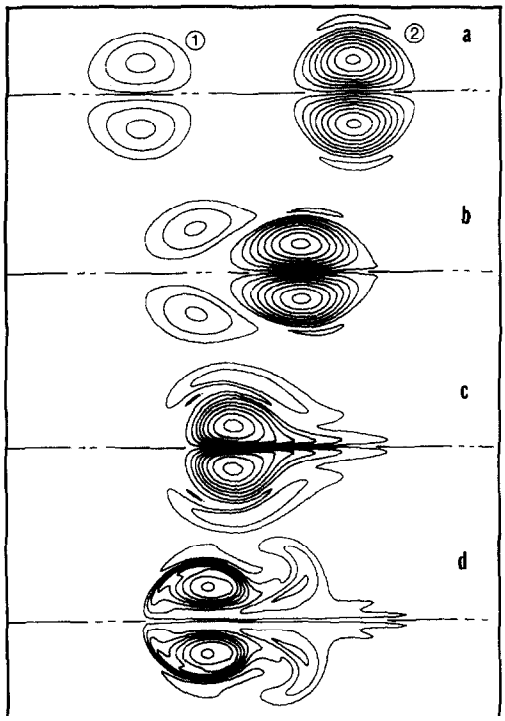
the experiment to numerical solutions of an initial-value problem on a periodic interval. They found the location and number of maxima (up to three) in one wavelength downstream from the wavemaker were in surprisingly good agreement. However, no comparison of absolute amplitudes could be made because they neglected dissipation. Hammack [148] and Hammack and Segur [149] continued with an impulsive wavemaker that generated an isolated waveform. In the latter, they used the inverse-scattering method for the KdV equation on the real line to predict the number of solitons to emerge from the initial waveform. For $50 < a\lambda^2/d^3 < 600$, the predicted number of emergent solitons was in agreement with experimental observations, but the predicted amplitude of the leading solitary entity differed by 15–20% from observed values, after a correction was made for damping. Further results on interacting localized waves were obtained by Weidman and Maxworthy [150].

To overcome the problems associated with using undamped, initial-value solutions, Bona, Pritchard and Scott [146] made a comprehensive and coordinated analytical, computational and experimental study. After a discussion of several models of damping, they "... decided to use and *ad-hoc* representation of the wave damping..." and numerically solved

$$\eta_t + \alpha\eta_x + \beta\eta\eta_x + \nu\eta - \mu\eta_{xx} - \gamma\eta_{xxt} = 0, \tag{96}$$

which is their Eq. (7.1) designated ($M\dagger$). They designed an explicit, unconditionally stable fourth-order space-time algorithm for the semi-infinite line with a time-dependent boundary condition (that simulates the wavemaker). They developed a novel numerical procedure, analyzed discretization errors, and examined convergence. If we set the two damping constants $\nu = \mu = 0$ and $\alpha = 1$, $\beta = \frac{3}{2}$ and $\gamma = \frac{1}{6}$, Eq. (96) becomes the RLW equation obtainable by an asymptotic procedure from the incompressible Euler equations.

In their computational–experiment comparisons they found quantitative agreement for $S \leqslant 11.8$ and $\alpha = 1$, $\beta = \frac{3}{2}$, $\gamma = \frac{1}{6}$, $\nu = 0$, $\mu = 0.014$. However, for $S = 18.1$, the agreement between computation and experiment was "... significantly worse..." than in earlier cases (as shown in their Fig. 9) "... for the experimental results indicate the presence of a substantial amount of second-harmonic component which is not nearly so strongly evident in the theoretical solutions of Fig. 11b." They assess all the possible causes and decide that by "... tinkering with the model the agreement could be improved" [151]. In essence, they varied the parameters in (96) to be consistent with a linear dispersion relation that includes a bottom boundary layer for dissipation. Still, they found that the model did not yield quantitative comparisons for $S \geqslant 26.3$. "... At larger values of S their were features of the experiments [higher harmonics] that were not predicted by the model." The disagreement probably arose because of the large effective damping coefficient of the experimental environment. That is, the tank constraints caused them to operate with a small still water depth and a small wavelength. This made the damping term μu_{xx} and the dispersive term γu_{xxt} of *comparable* magnitude. This is readily seen in their Figs. 11a and 16, which give the waveform of $\eta(x, t)$ at a given large time. One sees a high harmonic content near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of our consciousness. To date, and for many, deductive mathematics has often bridged the two domains. A proper picture or graph in the external domain can synergize the formation of images in our "nonconscious" mind and provide an alternative circuit for discovery. Many present abstract fields of mathematics had their origin in making this linkage.

With computers, the intuitive–geometric approach can be developed, taught to our students and made part of the scientists *modus operandi.*

APPENDIX A. Excerpt from Pamphlet Accompanying the Soliton Film Describing Solution of the Modified KdV Equation [41].

Part II. Interaction of a Compressive and Rarefactive Soliton; Numerical solutions of the partial differential equation

$$u_t + u^2 u_x + \delta^2 u_{xxx} = 0 \qquad (0 \leqslant x \leqslant 2), \tag{A1}$$

with periodic boundary conditions (December, 1965).

For the numerical simulation of (A1), the interval $0 \leqslant x \leqslant 2$ was divided into 400 positions x_ν and the equation was discretized in the variables x and t according to the *explicit* scheme:

$$\begin{aligned} u(x_\nu, t + \tfrac{1}{4}\Delta t) &= u(x_\nu, t) - \tfrac{1}{2}\mathscr{F}_\nu[u, t], \qquad t = 0, \tfrac{1}{4}\Delta t, \tfrac{1}{2}\Delta t, \tfrac{3}{4}\Delta t; \\ u(x_\nu, t + \Delta t) &= u(x_\nu, t - \Delta t) - \mathscr{F}_\nu[u, t], \qquad t = \Delta t, 2\Delta t, \ldots; \end{aligned} \tag{A2}$$

where

$$\mathscr{F}_\nu[u, t] = \tfrac{1}{6}\frac{\Delta t}{\Delta x}\left[\frac{u^4(x_{\nu+1}, t) - u^4(x_\nu, t)}{u(x_{\nu+1}, t) - u(x_\nu, t)} - \frac{u^4(x_\nu, t) - u^4(x_{\nu-1}, t)}{u(x_\nu, t) - u(x_{\nu-1}, t)}\right]$$
$$+ 2\delta^2 \frac{\Delta t}{(\Delta x)^3}\left[u(x_{\nu+2}, t) - 2u(x_{\nu+1}, t) + 2u(x_{\nu-1}, t) - u(x_{\nu-2}, t)\right], \tag{A3}$$

and

$$\Delta x = 0.005, \qquad \Delta t = 1.155 \times 10^{-4}, \qquad \delta = 0.0208.$$

The initial condition is

$$u(x_\nu, 0) = A_1 \operatorname{sech}[(6^{-1/2}A_1/\delta)(x_\nu - x_{10})] + A_2 \operatorname{sech}[(6^{-1/2}A_2/\delta)(x_\nu - x_{20})], \tag{A4}$$

where

$$A_1 = 1.0, \qquad A_2 = -0.667, \qquad x_{10} = 0.45, \qquad x_{20} = 1.0.$$

The calculation was carried to 87,000 computation steps ($t = 10.50$), at which time the two solitons have completed their interaction. The film has a frequency of one

frame every 15 computation steps. At the end of Part II, the rarefactive soliton reenters the spatial (x) interval from the left as a result of the periodic boundary conditions.

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The developments described in Section 3 owe much to Martin David Kruskal's genuine warmth and friendliness to neophyte scientists, his deep insight and his power with asymptotics.

This paper grew out of a talk, "Computational Synergetics: The Way to the Soliton and Beyond"(unpublished) that I was privileged to give at the Second International Soliton Workshop in Jadwisin, Poland, August 1979. This paper was written while I visited the Laboratory of Applied Mathematical Physics at the Technical University of Denmark. The hospitality, discussions and support of the scientists and staff made the task easier. Particularly, I am grateful to O. Skovgaard, who supplied me with reference material from his extensive library. I am also grateful to F. Calogero, J. Ford, R. Hermann, J. W. Miles, and V. G. Makhankov for their valuable comments on a preliminary version of this paper.

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   When faced with a complex and highly tangled mathematical representation, as almost all

nonlinear problems are, one uses the computer as an heuristic probe, to force an opening into a region of difficulty. The numerical "answers" to this problem, if properly assimilated, can provide the prepared investigator with a new level of insight which may permit him to resolve an area of trouble by conventional analysis—usually some form of uniform asymptotic analysis, and rarely an exact solution, In attempting to complete this analysis or understand completely the details of the computer solution, the investigator will uncover a group of problems which will lead him further into the maze. Oftentimes he will have to back away from an impasse, review the problem, and probe another aspect of the equations. He must be constantly on the lookout for the new and small phenomena generated by the computer, for an understanding of these often will provide the pathways to an eventual analytical and global understanding of the properties of his equations."

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